

CogDL: A Toolkit for Deep Learning on Graphs

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Abstract—Deep learning on graphs has attracted tremendous attention from the graph learning community in recent years. It has been widely adopted in various real-world applications from diverse domains, such as social and information networks, biological graphs, and molecular graphs. In this paper, we present CogDL—an extensive toolkit for deep learning on graphs—that allows researchers and developers to easily conduct experiments and build applications. In CogDL, we propose a unified design for the training loop of graph neural network (GNN) models, making it unique among existing graph learning libraries. By utilizing this unified trainer, we can optimize the GNN training loop with several training techniques such as distributed training and mixed precision training. Moreover, we develop efficient sparse operators for CogDL, enabling it to become the most competitive graph library for efficiency. Additionally, another important CogDL feature is its focus on ease of use with the goal of facilitating open, robust, and reproducible graph learning research. We leverage CogDL to report and maintain benchmark results on the fundamental graph tasks such as node classification and graph classification, which can be reproduced and directly used by the community. Finally, we demonstrate the effectiveness and efficiency of CogDL for real-world applications in AMiner—a large-scale academic mining and search system. The CogDL toolkit is available at: <https://github.com/thudm/cogdl>.

Index Terms—Graph representation learning, Graph neural networks, Frameworks.



1 INTRODUCTION

Graph-structured data have been widely utilized in many real-world scenarios. Inspired by recent trends of representation learning on computer vision and natural language processing, graph representation learning [1, 2, 3] is proposed as a powerful technique to handle the graph-structured data. Representation learning on graphs aims to learn low-dimensional continuous vectors for graph objects, such as vertices and sub-graphs, while preserving intrinsic graph properties.

Broadly, the graph representation learning methods can be classified into two categories. One type of them, network embedding, focuses on designing strategies to project (only) graph structures into the latent space, that is, encoding structural properties into embeddings. Notably, the skip-gram [4] based methods pioneer the study of network embedding. Take DeepWalk [1] for example, it transforms the graph structure into a uniformly sampled collection of truncated random walks and optimizes with the skip-gram model, which further inspires the node2vec [3] and meta-

path2vec [5] methods. A later study shows that this set of techniques—random walk and skip-gram—is theoretically equivalent to implicit matrix factorization, based on which the NetMF method [6] is proposed to factorize a proximity matrix for generating network embeddings. This direction is further extended by sparse matrix factorization techniques, enabling efficient embedding learning for billion-scale networks [7, 8].

Graph neural networks (GNNs) [9, 10], as the other major type of graph representation learning methods, apply neural architectures to perform message passing over graph structures. Thus, the input to GNNs usually contains both structural information and graph feature information, such as node and edge features. For example, graph convolution networks (GCNs) [11] utilize a convolutional architecture via a localized first-order approximation of spectral graph convolutions. GraphSAGE [12] is a general inductive framework that leverages node features to generate node embeddings for previously unseen nodes. Recent effort in GNNs has been focused on its theoretical understanding [13], generalization [14], self-supervised learning [15, 16], and capacity of handling Web-scale applications [17]. To date, GNNs have achieved impressive performance on various graph machine learning tasks in diverse domains [18].

The progress of graph representation learning has largely benefited from the advances in deep learning in natural language processing and computer vision. However, the graph-structured data is fundamentally different with natural language or images, which can be easily formatted as *Tensor* and thus straightforwardly processed by GPUs. The non-Euclidean and sparse nature of graph data requires a better storage format for efficient computation especially on GPUs. However, current Deep Learning frameworks do not well support the sparse computation of graph-

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TABLE 1: Overview of current GNN toolkits.

	Backend	Graph Class	Operator Acceleration	Reproducible Configuration	Hyperparameter Optimization	Unified Trainer
ptggn ¹	PyTorch	GraphData	–	–	–	–
PGL ²	PaddlePaddle	Graph	–	–	–	–
Eular ³	TF	DataSet	–	–	–	–
Graph Nets [19]	TF1	GraphsTuple	–	–	–	–
Jraph [20]	JAX	GraphsTuple	–	–	–	–
Graph-Learn [21]	PyTorch/TF	Graph	–	–	–	–
Spektral [22]	TF2/Keras	Graph	–	–	–	–
StellarGraph [23]	TF2/Keras	StellarGraph	–	–	–	–
DGL [24]	PyTorch/TF2/MXNet	DGLGraph	✓	✓	–	–
PyG [25]	PyTorch	Data/HeteroData	✓	✓*	✓*	–
CogDL	PyTorch	Graph	✓	✓	✓	✓

¹ <https://github.com/microsoft/ptggn>

² <https://github.com/PaddlePaddle/PGL>

³ <https://github.com/alibaba/euler>

* PyG 2.0 utilizes GraphGym [26] for the two features.

structure data. For example, the PyTorch API of sparse tensors is limited and inefficient for graph operations. To bridge the gap, several open-source effort has been made to develop dedicated toolkits for efficient developments of graph representation learning research. We summarize the characteristics of existing graph toolkits in Table 1. Among them, the PyTorch Geometric (PyG) [25] and Deep Graph Library (DGL) [24] are two of the most well-known libraries with efficient operators and easy-to-use APIs.

PyG is a graph learning library built upon PyTorch [27] to easily write and train GNNs for a wide range of applications related to structured data. PyG achieves high data throughput by leveraging sparse GPU acceleration and by providing dedicated CUDA kernels. PyG 2.0 further utilizes GraphGym [26] to achieve new features like reproducible configuration and hyperparameter optimization. DGL is an efficient and scalable package for deep learning on graphs, which provides several APIs allowing arbitrary message-passing computation over large-scale graphs with efficient memory usage and high training speed. Besides, DGL allows users to easily port and leverage the existing components across multiple deep learning frameworks (e.g., PyTorch, TensorFlow, MXNet). However, these popular graph libraries mainly focus on implementing GNN layers/models and do not provide a unified trainer for the GNN training. Users need to write tedious code to build a complete loop for GNN model training and evaluation, such as early stopping, model saving, and experiment logging.

Present work: CogDL. In this paper, we introduce CogDL¹, an extensive graph representation learning toolkit that allows researchers, practitioners, and developers to easily conduct experiments and build large-scale applications. The advantage of CogDL lies in its design of a unified GNN trainer and modular wrappers. Specifically, CogDL unifies the training loop of graph neural network (GNN) models, making it different from other graph learning libraries. In addition, it is also equipped with decoupled modules that can be flexibly plugged for training GNNs, including *Model Wrapper* and *Data Wrapper*.

Based on the design of the unified trainer and decoupled modules, CogDL users can easily instantiate a GNN trainer by `trainer = Trainer(...)` and then call `trainer.run(...)` to conduct experiments, which is not supported by existing libraries. Figure 1 illustrates the benefits of CogDL’s unified trainer and modular wrappers over PyG and DGL. By using this unified trainer, it not only saves users’ time of writing additional code, but also gives users the opportunities to enable many built-in training techniques such as mixed precision training. For example, users only need to set `Trainer(fp16=True)` to enable the feature of mixed precision training without any modification.

We summarize the characteristics of CogDL as follows:

- **A Unified Trainer.** CogDL integrates a unified trainer with decoupled modules for the GNN training. Based on this unique design, CogDL can provide extensive features such as hyperparameter optimization, distributed training, training techniques, and experiment management.
- **Efficient Sparse Operators.** Efficiency is one of the most significant characteristics of CogDL. CogDL develops well-optimized sparse kernel operators to speed up the training of GNN models. For example, these efficient sparse operators enable CogDL to achieve about 2× speedups on the 2-layer GCN [11] and GAT [28] models compared with PyG and DGL.
- **Ease of Use.** We provide simple APIs in CogDL such that users only need to write one line of code to train and evaluate any graph representation learning methods. In addition, CogDL also collects and maintains the state-of-the-art configurations of 60+ models on 40+ public datasets, facilitating open, robust, and reproducible deep learning research on graphs.

2 COGDL: OVERVIEW

The goal of CogDL is to accelerate research and applications of deep learning on graphs. CogDL provides a novel and unified training loop for GNN models, which is quite different from other graph learning libraries. Based on the unified GNN training, CogDL optimizes the training with several efficient techniques and well-optimized sparse operators. Furthermore, we provide essential experimental results reproduced by CogDL with hyperparameter configurations.

1. The toolkit is available at: <https://github.com/thudm/cogdl>

	CogDL	PyG	DGL
1	<code>model = GCN(...)</code>	<code>model = GCN(...)</code>	<code>model = GCN(...)</code>
2	<code>data = CoraDataset()[0]</code>	<code>data = Planetoid(name="Cora")[0]</code>	<code>data = CoraGraphDataset()[0]</code>
3	<code>mw = ModelWrapper(model, ...)</code>	<code>optimizer = torch.optim.Adam(...)</code>	<code>optimizer = torch.optim.Adam(...)</code>
4	<code>dw = DataWrapper(data, ...)</code>	<code>for epoch in range(100):</code>	<code>for epoch in range(100):</code>
5	<code>trainer = Trainer(epochs=100)</code>	<code>pred = model(data.x, data.edge_index)</code>	<code>pred = model(data)</code>
6	<code>result = trainer.run(mw, dw)</code>	<code>labels = data.y</code>	<code>labels = data.ndata['label']</code>
7		<code>mask = data.train_mask</code>	<code>mask = data.ndata['train_mask']</code>
8		<code>loss = F.nll_loss(pred[mask],</code>	<code>loss = F.nll_loss(pred[mask],</code>
9		<code>labels[mask])</code>	<code>labels[mask])</code>
10		<code>optimizer.zero_grad()</code>	<code>optimizer.zero_grad()</code>
11		<code>loss.backward()</code>	<code>loss.backward()</code>
12		<code>optimizer.step()</code>	<code>optimizer.step()</code>
13		<code>val_acc = evaluate(model, data)</code>	<code>val_acc = evaluate(model, data)</code>
14		<code>if val_acc > best_val_acc:</code>	<code>if val_acc > best_val_acc:</code>
15		<code>best_val_acc = val_acc</code>	<code>best_val_acc = val_acc</code>
16		<code>best_model = deepcopy(model)</code>	<code>best_model = deepcopy(model)</code>
17		<code>result = test(best_model, data)</code>	<code>result = test(best_model, data)</code>

Fig. 1: Illustration of training the GCN model on the Cora dataset using CogDL, PyG, and DGL. The trainer of CogDL takes over the entire loop of the training process. The model wrapper consists of the training and testing steps, while the data wrapper handles the data preparation and transformation.

In the subsequent sections (Sections 3, 4, and 5), we describe each characteristic of CogDL in detail. CogDL provides accelerated sparse operators and reproducible hyperparameter configurations like PyG and DGL. Besides, CogDL offers native support for hyperparameter optimization, which PyG supports it via GraphGym. In addition, the design of the unified trainer is the most impressive contribution of CogDL. The advantages of the unified trainer will be introduced in Section 3. Section 4 introduces the performance of efficient operators implemented in CogDL.

In Section 5, we give the experimental results reproduced by CogDL to cover the widely used settings. Although there are enormous research works on graph machine learning, we find that different papers may use their own evaluation settings for the same graph dataset, making results indistinguishable. For example, as a widely used dataset, Cora [29], some papers use the “standard” semi-supervised splits following Planetoid [30], while others adopt random splits or fully-supervised splits. Reported results of the same model on the same dataset may differ in various papers, making it challenging to compare performance reported across various studies [18, 31, 32, 33].

In Section 6, we introduce the main elements and usages of CogDL. CogDL provides easy-to-use APIs for conducting experiments and building applications. Finally, in Section 7, we introduce some real-world applications built on CogDL. We demonstrate how CogDL supports academic applications, including paper tagging and recommendation.

3 THE COGDL FRAMEWORK

In this section, we present the design of CogDL framework, as shown in Figure 2. Our framework is built on PyTorch [27], which is the most popular deep learning library. PyTorch provides an imperative and Pythonic programming style that supports code as a model and makes debugging easy. Therefore, our toolkit can leverage the advantages of PyTorch. CogDL provides implementations of many models such as GCN and GAT, based on PyTorch and our own

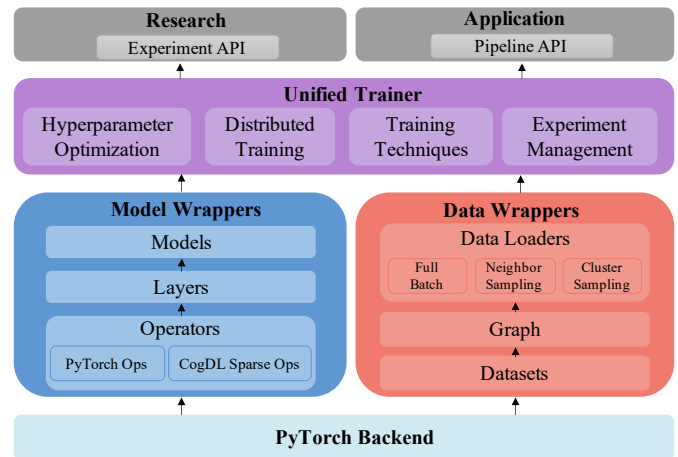


Fig. 2: Overview of the CogDL framework. CogDL develops a unified trainer with decoupled modules, which unifies the training loop for GNN models. The model wrapper provides functions of training and testing steps called by the trainer, while the data wrapper offers training and testing data loaders for the model wrapper. Besides, CogDL develops efficient sparse operators related to graph operations such as Sparse Matrix Multiplication (SpMM). Based on these operators, CogDL implements dozens of graph representation models. CogDL integrates different types of real-world graph datasets, including social networks, molecular graphs, academic graphs, etc. All these models and datasets can be utilized for various downstream tasks.

sparse operators. It also supports several genres of datasets for graph tasks such as node classification and graph classification. All the models and datasets are compatible with our unified trainer for experiments.

3.1 Unified Trainer

CogDL provides a unified trainer for GNN models, which takes over the entire loop of the training process. The unified

TABLE 2: Decoupled modules for representative GNNs. The model wrapper (MW) is for training and testing steps. The data wrapper (DW) is for constructing data loaders.

	model	MW	DW
GCN [11]	GCN	supervised	full-graph
GraphSAGE [12]	SAGE	sage_mw ¹	neighbor sampling
Cluster-GCN [34]	GCN	supervised	clustering
DGI [15]	GCN	dgi_mw ²	full-graph

¹ GraphSAGE uses random-walk-based unsupervised loss.

² DGI uses local-global mutual information loss.

trainer, which contains much engineering code, is implemented flexibly to cover arbitrary GNN training settings. We design four decoupled modules for the GNN training, including *Model*, *Model Wrapper*, *Dataset*, *Data Wrapper*. The *Model Wrapper* is for the training and testing steps, while the *Data Wrapper* is designed to construct data loaders used by *Model Wrapper*. The main contributions of most GNN papers mainly lie on three modules except *Dataset*, as shown in Table 2. For example, the GCN paper trains the GCN model under the (semi-)supervised and full-graph setting, while the DGI paper trains the GCN model by maximizing local-global mutual information. The training method of the DGI is considered as a model wrapper named *dgi_mw*, which could be used for other scenarios.

Based on the design of the unified trainer and decoupled modules, we could do arbitrary combinations of models, model wrappers, and data wrappers. For example, if we want to apply DGI to large-scale datasets, all we need is to substitute the full-graph data wrapper with the neighbor-sampling or clustering data wrappers without additional modifications. If we propose a new GNN model, all we need is to write essential PyTorch-style code for the model. The rest could be automatically handled by CogDL by specifying the model wrapper and the data wrapper. We could quickly conduct experiments for the model using the trainer via *trainer = Trainer(epochs,...)* and *trainer.run(...)*. Moreover, based on the unified trainer, CogDL provides native supports for many useful features, including hyperparameter optimization, distributed training, training techniques, and experiment management without any modification to the model implementation.

3.2 Training Techniques

We introduce training techniques of GNN training, which credit to the unified trainer of CogDL. These features could be enabled through *fp16=True* or *actnn=True* in the *Experiment* API, which will be introduced in Section 6.

TABLE 3: Performance of mixed precision training.

	Memory	Accuracy	Training Speed	
			2080 Ti	3090
w/o fp16	5,567 MB	95.44	2.20 it/s	3.93 it/s
with fp16	4,046 MB	95.35	3.17 it/s	7.97 it/s

Mixed Precision Training. We also support mixed precision training which is a popular technique to relieve the GPU memory and speed up the training process. PyTorch

provides a convenience method for mixed precision in *torch.cuda.amp*, which integrates NVIDIA apex. For example, we conduct experiments for testing the performance of mixed precision training. We run a 2-layer GCN model with 2048 hidden units on the Reddit dataset. From Table 3, the mixed precision training brings 27% memory savings and $1.44\times \sim 2.02\times$ speedup on NVIDIA 2080 Ti and 3090 GPUs.

TABLE 4: Accuracy (%) and activation memory (MB) of 2-layer GCNs on three datasets.

	origin (32bit)	actnn (4bit)	actnn (3bit)	actnn (2bit)
Flickr	51.17 (288)	51.08 (33)	51.14 (28)	51.20 (20)
Reddit	95.33 (1532)	95.32 (209)	95.31 (159)	95.34 (121)
Yelp	40.05 (4963)	40.47 (825)	40.14 (693)	37.68 (571)

Activation Compression Training. As the emergence of deep GNNs, the activation footprints occupy more and more GPU memory. And we need to store the activation output of each layer to compute the gradient in the backward pass, which costs much GPU memory in the training step. We extend the activation compression training (actnn) [35] to GNNs. The main advantage of activation compression training is that the GPU memory of training could dramatically decrease. We conduct experiments of the 2-layer GCN model on three datasets for the activation compression training in the CogDL, as shown in Table 4. The performance demonstrates that training GNNs with actnn brings $6.0\times \sim 14.4\times$ memory savings, compared with 32-bit training. The accuracy with actnn is almost the same with 32-bit training except the accuracy (37.68) on Yelp with 2-bit actnn. In real cases, we could choose a proper compression bit to enjoy memory savings with few performance drop.

3.3 Distributed Training

Large-scale graph training often depends on sampling based methods, such as GraphSAGE and ClusterGCN. We further speed up the mini-batch training via PyTorch distributed data parallel (DDP). CogDL has implemented distributed training of commonly used sampling methods, including GraphSAGE and ClusterGCN. We conduct experiments of GraphSAGE and ClusterGCN on Reddit datasets via 2080 Ti. The training time of ClusterGCN is 0.63, 0.33 ($1.91\times$), 0.20 ($3.15\times$) seconds per epoch for 1, 2, 4 GPUs, respectively. Meanwhile, the training time of GraphSAGE is 4.35, 2.44 ($1.78\times$), 1.22 ($3.57\times$) seconds per epoch for 1, 2, 4 GPUs, respectively. The results demonstrate the near-linear acceleration for distributed training of CogDL.

3.4 Hyperparameter Optimization

Hyperparameter optimization (HPO) is an important feature for GNN libraries, since current GNN models utilize more hyperparameters than before. We integrate a popular library, Optuna [36] into CogDL to enable HPO. Optuna is a fast AutoML library based on Bayesian optimization. CogDL implements hyperparameter search and even model search for graph learning. The key of the HPO is to define a search space. The search space will be automatically utilized by CogDL to start searching and output the best results. The usage of HPO could be found in Section 6.1.

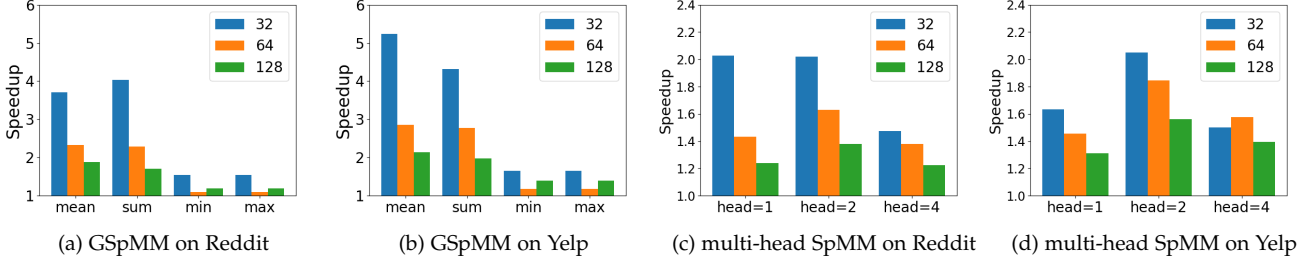


Fig. 3: Speedup of GSpMM and multi-head SpMM operators with 32, 64, 128 hidden units compared with DGL. (a) $1.70\times \sim 4.04\times$ speedup with mean and sum as reduce functions on Reddit. (b) $1.98\times \sim 5.24\times$ speedup with mean and sum as reduce functions on Yelp. (c) $1.22\times \sim 2.03\times$ speedup with 1, 2, 4 attention heads on Reddit. (d) $1.31\times \sim 2.05\times$ speedup with 1, 2, 4 attention heads on Yelp.

3.5 Experiment Management

The experiment management is crucial for training deep learning models, which could be utilized by researchers and developers for debugging and designing new blocks. We provide two kinds of loggers for experiment management, including TensorBoard and WandB [37]. TensorBoard is a common visualization toolkit for tracking metrics like loss and accuracy. WandB is a central dashboard to keep track of experimental status. The experiment management could be enabled easily by assigning the *logger* argument.

4 EFFICIENCY OF COGDL

In this section, we introduce the well-optimized sparse operators, including SpMM-like operators, multi-head SpMM, and edge-wise softmax, which are developed and implemented in CogDL for GNN models.

Graph Notations. Denote a network $G = (V, E)$, where V is a set of n nodes and $E \subseteq V \times V$ is a set of edges between nodes. Each node v may be accompanied with its feature x_v . We use A to denote the adjacency matrix (binary or weighted), and D to denote the diagonal degree matrix, with $D_{ii} = \sum_j A_{ij}$. Each edge $e_{ij} = (v_i, v_j)$, associated with a weight $A_{ij} \geq 0$, indicates the strength of the relationship between v_i and v_j . In practice, the network could be either directed or undirected. If G is directed, we have $A_{ij} \neq A_{ji}$ and $e_{ij} \neq e_{ji}$. if G is undirected, we have $e_{ij} = e_{ji}$ and $A_{ij} = A_{ji}$.

4.1 Efficient Sparse Operators

We first introduce an important operator used in CogDL and its corresponding optimization. The General Sparse Matrix-Matrix multiplication (GSpMM) operator is widely used in most of GNNs. The reason is that many GNNs apply an general aggregation operation for a given node from nodes of its incoming edges:

$$\mathbf{h}_u^{(l+1)} = \phi(\psi(\mathbf{h}_v^{(l)}, \mathbf{h}_e)), v \in \mathcal{N}(u), e = (u, v) \in E, \quad (1)$$

where $\mathcal{N}(u)$ is the set of neighbors of node u , $\mathbf{h}_u^{(l)}$ is the representation vector of node u of layer l . When ϕ , the reduce operation is a summation, and ψ , the compute operation is a multiplication, such an operation can be described as an

SpMM operator $\mathbf{H}^{(l+1)} \leftarrow \mathbf{A}\mathbf{H}^{(l)}$, where the sparse matrix A represents the adjacency matrix of the input graph G , and each row of $\mathbf{H}^{(l)}$ represents a representation vector of nodes (e.g., $\mathbf{h}_u^{(l)}$ and $\mathbf{h}_v^{(l)}$). Many previous works focused on improving the performance of executing the SpMM operator on GPUs, such as ASpT [38], GraphBlast [39] and GE-SpMM [40]. We design GSpMM for our CogDL toolkit by extending the design methodology of GE-SpMM [40]. Compared with of PyG based on the COO-format design, CogDL utilizes CSR-format design, making aggregation process as a whole SpMM function. Also, by using our GSpMM, users could choose the reduce or compute operator as illustrated in Equation 1.

This abstraction of our GSpMM is similar to DGL and we will further describe our superiority in kernel design. Compared with DGL, our implementations are much more efficient due to our architecture-aware kernel design. In multi-head SpMM kernel, we apply the memory coalescing technique by allocating consecutive threads along the dimension of the feature. In this way, when threads within one warp access different features of the same vertex, their memory access will be combined into one single transaction and the memory bandwidth will be saved. We also allocate consecutive warps along the dimension of the head. As different heads share the same location of non-zero elements, this data will be cached by the streaming multiprocessors and reused among different heads, which also saves bandwidth. In our GSpMM design, we implement a shared memory method to cache those data for edge weight and column indices. We conducts experiments of GSpMM and multi-head SpMM on Reddit and Yelp datasets compared to DGL, as shown in Figure 3. For GSpMM, CogDL achieves $1.70\times \sim 5.24\times$ speedup with mean and sum as reduce functions and $1.10\times \sim 1.66\times$ speedup with min and max as reduce functions. For multi-head SpMM, CogDL achieves $1.22\times \sim 2.03\times$ and $1.31\times \sim 2.05\times$ speedup on Reddit and Yelp datasets, respectively.

When considering a GAT model, we also need a sampled dense-dense matrix multiplication (SDDMM) operator $\mathbf{T} = \mathbf{A} \odot (\mathbf{P}\mathbf{Q}^T)$, where \mathbf{T} and \mathbf{A} are the sparse matrices, \mathbf{P} and \mathbf{Q} are two dense matrices, \odot is element-wise matrix multiplication. The SDDMM operator is used for back-propagating the gradients to the sparse adjacency matrix since the adjacency matrix of the GAT model is computed by

the attention mechanism. CogDL further speeds up multi-head graph attention by optimizing Edge-wise Softmax, which is defined by $\alpha'_{uv} = \exp(\alpha_{uv}) / (\sum_{v \in \mathcal{N}(u)} \exp(\alpha_{uv}))$, where α_{uv} is the attention score of between nodes u and v . In our design of Edge-wise Softmax kernel, we used the method of warp level intrinsic provided by NVIDIA, a typical method that could accelerate the scan and reduce operation. To prevent from the spillover of exponent, we first apply the scan to find the max value of edge weight then subtract this maximum from each value. After that, we compute each value by applying the exponent function and reduce all the value within the warp to acquire the sum of all the exponent value.

TABLE 5: End-to-end inference time in seconds of 2-layer GCN and GAT models with hidden size 128. The GAT model uses 4 attention heads. OOM means out of memory.

Model	GPU	Dataset	PyG	DGL	CogDL
GCN	2080Ti (11G)	Flickr	0.004	0.007	0.004
		Reddit	0.045	0.049	0.039
		Yelp	0.053	0.063	0.042
	3090 (24G)	Flickr	0.002	0.004	0.002
		Reddit	0.023	0.031	0.022
		Yelp	0.029	0.036	0.023
GAT	2080Ti (11G)	Flickr	0.033	0.019	0.014
		Reddit	OOM	0.214	0.131
		Yelp	OOM	OOM	0.138
	3090 (24G)	Flickr	0.021	0.013	0.009
		Reddit	OOM	0.112	0.080
		Yelp	OOM	0.107	0.081

4.2 End-to-End Performance

We compare the end-to-end inference time of GCN and GAT models on several datasets with other popular GNN frameworks: CogDL v0.5.2, PyTorch-Geometric (PyG) v2.0.2, and Deep Graph Library (DGL) v0.7.2 with PyTorch backend. The statistics of datasets could be found in Table 6. We conduct experiments using Python 3.7.10 and PyTorch v1.8.0 on servers with Nvidia GeForce RTX 2080 Ti (11GB GPU Memory) and 3090 (24GB GPU Memory). From Table 5, CogDL achieves at most $2\times$ speedup on the 2-layer GCN model compared with PyG and DGL. For the 2-layer GAT model, CogDL achieves $1.32\times \sim 2.36\times$ speedup compared with PyG and DGL. Furthermore, OOM occurs when running the PyG’s GAT model on Reddit and Yelp datasets, even using 3090 (24G). The GAT model implemented by DGL also cannot run the Yelp dataset using 2080Ti (11G). The results demonstrate significant advantages of CogDL in inference time and memory savings, compared to state-of-the-art GNN frameworks.

5 EXPERIMENTS AND ANALYSES

In this section, with CogDL, we provide several downstream tasks including node classification and graph classification to evaluate implemented methods. We also build a reliable leaderboard for each task, which maintain benchmarks and state-of-the-art results on this task.

5.1 Unsupervised Node Classification

Unsupervised node classification task aims to learn a mapping function $f : V \mapsto \mathbb{R}^d$ that projects each node to a d -dimensional space ($d \ll |V|$) in an unsupervised manner. Structural properties of the network should be captured by the mapping function.

Datasets. We collect the most popular datasets used in the unsupervised node classification task. Table 6 shows the statistics of these datasets.

- BlogCatalog [44] is a social blogger network, where nodes and edges stand for bloggers and their social relationships, respectively. Bloggers’ interests are used as labels.
- Wikipedia² is a co-occurrence network of words in the first million bytes of the Wikipedia dump. The labels are the Part-of-Speech (POS) tags inferred by Stanford POS-Tagger [45].
- PPI [46] is a subgraph of the PPI network for Homo Sapiens. Node labels are extracted from hallmark gene sets and represent biological states.
- DBLP [47] is an academic citation network where authors are treated as nodes and their dominant conferences as labels.
- Flickr [48] is the user contact network between users in Flickr. The labels represent the interest groups of the users.

Models. We implement and compare the following methods for the unsupervised node classification task. These methods can be divided into two categories. One is Skip-gram based models, and the other is matrix factorization based models.

- SpectralClustering [41] generates node representations from the d -smallest eigenvectors of the normalized graph Laplacian.
- DeepWalk [1] transforms a graph structure into linear sequences by truncating random walks and processing the sequences using Skip-gram with hierarchical softmax.
- LINE [2] defines loss functions to preserve first-order or second-order proximity separately and concatenates two representations together.
- node2vec [3] designs a biased random walk procedure with Breadth-first Sampling (BFS) and Depth-first Sampling (DFS) to make a trade off between homophily similarity and structural equivalence similarity.
- GraRep [43] decomposes k -step probability transition matrix to train the node embedding, then concatenate all k -step representations.
- HOPE [42] approximates high-order proximity based on factorizing the Katz matrix.
- NetMF [6] shows that Skip-gram models with negative sampling like Deepwalk, LINE can be unified into the matrix factorization framework with closed forms.
- ProNE [7] firstly transforms the graph representation learning into decomposition of a sparse matrix, and further improves the performance through spectral propagation technology.
- NetSMF [8] addresses the efficiency and scalability challenges faced by the NetMF model via achieving a sparsification of the (dense) NetMF matrix.

2. <http://www.mattmahoney.net/dc/text.html>

TABLE 6: Dataset statistics for node classification (“m” stands for multi-label classification)

Setting	Dataset	#Nodes	#Edges	#Features	#Classes	# Train / Val / Test
Semi-supervised Setting	Cora	2,708	5,429	1,433	7	140 / 500 / 1,000
	Citeseer	3,327	4,732	3,703	6	120 / 500 / 1,000
	Pubmed	19,717	44,338	500	3	60 / 500 / 1,000
Fully-Supervised Setting	PPI	56,944	818,736	50	121 (m)	0.79 / 0.11 / 0.10
	Flickr	89,350	899,756	500	7	0.50 / 0.25 / 0.25
	Reddit	232,965	11,606,919	602	41	0.66 / 0.10 / 0.24
	Yelp	716,847	6,977,410	300	100 (m)	0.75 / 0.10 / 0.15
	ogbn-arxiv	169,343	1,166,243	128	40	0.54 / 0.18 / 0.28
Unsupervised Setting	PPI	3,890	76,584	-	50 (m)	0.50 / - / 0.50
	Wikipedia	4,777	184,812	-	40 (m)	0.50 / - / 0.50
	Blogcatalog	10,312	333,983	-	39 (m)	0.50 / - / 0.50
	DBLP	51,264	127,968	-	60 (m)	0.05 / - / 0.95
	Flickr	80,513	5,899,882	-	195 (m)	0.05 / - / 0.95

TABLE 7: Micro-F1 score (%) reproduced by CogDL for unsupervised multi-label node classification, including matrix factorization and skip-gram methods. 50% of nodes are labeled for training in PPI, Blogcatalog, and Wikipedia, 5% in DBLP and Flickr. These datasets correspond to different downstream scenarios: PPI stands for protein-protein interactions; Wikipedia is a co-occurrence network of words; Blogcatalog and Flickr are social networks; DBLP is a citation network.

Rank	Method	PPI (50%)	Wikipedia (50%)	Blogcatalog (50%)	DBLP (5%)	Flickr (5%)	Reproducible
1	NetMF [6]	23.73 ± 0.22	57.42 ± 0.56	42.47 ± 0.35	56.72 ± 0.14	36.27 ± 0.17	Yes
2	ProNE [7]	24.60 ± 0.39	56.06 ± 0.48	41.16 ± 0.26	56.85 ± 0.28	36.56 ± 0.11	Yes
3	NetSMF [8]	23.88 ± 0.35	53.81 ± 0.58	40.62 ± 0.35	59.76 ± 0.41	35.49 ± 0.07	Yes
4	Node2vec [3]	20.67 ± 0.54	54.59 ± 0.51	40.16 ± 0.29	57.36 ± 0.39	36.13 ± 0.13	Yes
5	LINE [2]	21.82 ± 0.56	52.46 ± 0.26	38.06 ± 0.39	49.78 ± 0.37	31.61 ± 0.09	Yes
6	DeepWalk [1]	20.74 ± 0.40	49.53 ± 0.54	40.48 ± 0.47	57.54 ± 0.32	36.09 ± 0.10	Yes
7	SpectralClustering [41]	22.48 ± 0.30	49.35 ± 0.34	41.41 ± 0.34	43.68 ± 0.58	33.09 ± 0.07	Yes
8	Hope [42]	21.43 ± 0.32	54.04 ± 0.47	33.99 ± 0.35	56.15 ± 0.22	28.97 ± 0.19	Yes
9	GraRep [43]	20.60 ± 0.34	54.37 ± 0.40	33.48 ± 0.30	52.76 ± 0.42	31.83 ± 0.12	Yes

Skip-gram network embedding considers the vertex paths traversed by random walks over the network as the sentences and leverages Skip-gram for learning latent vertex representation. For matrix factorization based methods, they first compute a proximity matrix and perform matrix factorization to obtain the embedding. Actually, NetMF [6] has shown the aforementioned Skip-gram models with negative sampling can be unified into the matrix factorization framework with closed forms.

Results and Analysis. We build a leaderboard for the unsupervised multi-label node classification setting. We run all algorithms on several real-world datasets and report the sorted experimental Micro-F1 results (%) using logistic regression with L2 normalization. Table 7 shows the results and we find some interesting observations.

- *Matrix factorization vs Skip-gram.* The leaderboard demonstrates that matrix factorization (MF) methods like NetMF and ProNE are very powerful and full of vitality as they outperform Skip-gram based methods in almost all datasets. ProNE and NetSMF are also of high efficiency and scalability and able to embed super-large graphs in feasible time in one single machine. There are many ways to further optimize these matrix related operations. The main advantage of Skip-gram methods is that they have good parallelism and are of high online while MF needs to recompute the embedding when the network changes.
- *Exploring neighborhoods.* Exploring a node’s network neighborhood is important in network embedding. DeepWalk and node2vec consider vertex paths traversed by random walk to reach high-order neighbors. NetMF and

NetSMF factorize diffusion matrix $\sum_{i=0}^K \alpha_i \mathbf{A}^i$ rather than adjacency matrix \mathbf{A} . ProNE and LINE are essentially 1-order methods, but ProNE further propagates the embeddings to enlarge the receptive field. Incorporating global information can improve performance but may hurt efficiency. The propagation in ProNE, which is similar to graph convolution, shows that incorporating global information as a post-operation is effective. In our experiments, stacking propagation on existing methods really improves its performance on downstream tasks.

TABLE 8: Accuracy (%) reproduced by CogDL for semi-supervised and self-supervised node classification on Citation datasets. ↓ and ↑ mean our results are lower or higher than the result in original papers. *Repro** is short for *Reproducible*.

Rank	Method	Cora	Citeseer	Pubmed	Repro*
1	GRAND [14]	84.8	75.1	82.4	Yes
2	GCNII [49]	85.1	71.3	80.2	Yes
3	MVGRL [50]	83.6 ↓	73.0	80.1	Partial
4	APNP [51]	84.3 ↑	72.0	80.0	Yes
5	Graph-Unet [52]	83.3 ↓	71.2 ↓	79.0	Partial
6	GDC [53]	82.5	72.1	79.8	Yes
7	GAT [28]	82.9	71.0	78.9	Yes
8	DropEdge [54]	82.1	72.1	79.7	Yes
9	GCN [11]	81.5	71.4 ↑	79.5	Yes
10	DGI [15]	82.0	71.2	76.5	Yes
11	JK-net [55]	81.8	69.5	77.7	Yes
12	Chebyshev [56]	79.0	69.8	68.6	Yes

5.2 Node Classification with GNNs

This task is for node classification with GNNs in semi-supervised and self-supervised settings. Different from the previous part, nodes in these graphs, like Cora and Reddit, have node features and are fed into GNNs with prediction or representation as output. Cross-entropy loss and contrastive loss are set for semi-supervised and self-supervised settings, respectively. For evaluation, we use prediction accuracy for multi-class and micro-F1 for multi-label datasets.

Datasets. The datasets consist of two parts, including both semi-supervised and fully-supervised settings.

- Semi-supervised datasets include three citation networks, Citeseer, Cora, and Pubmed [29]. These datasets contain sparse bag-of-words feature vectors for each document and a list of citation links between documents. We treat the citation links as (undirected) edges and construct a binary, symmetric adjacency matrix \mathbf{A} . Each document has a class label. For training, we only use 20 labels per class, but all feature vectors.
- Fully-supervised datasets include social networks (Reddit, Yelp, and Flickr), bioinformatics (PPI) from GraphSAINT [57], and ogbn-arxiv [18]. Reddit contains posts belonging to different communities with user comments. Flickr categorizes types of images based on the descriptions and common properties of online images and Yelp categorizes types of businesses based on customers, reviewers, and friendship. PPI aims to classify protein functions across various biological protein-protein interaction graphs. ogbn-arxiv is to predict the 40 subject areas of arXiv CS papers.

Models. GCNs [11] extend the convolution operation into graph-structured data by applying layer-wise propagation rule:

$$\mathbf{H}^{(l+1)} = \sigma(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}^{(l)}), \quad (2)$$

where $\hat{\mathbf{A}} = \tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}$ is the normalized adjacency matrix, $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}_n$ is the adjacency matrix with augmented self-connections, \mathbf{I}_n is the identity matrix, $\tilde{\mathbf{D}}$ is the diagonal degree matrix where $\tilde{\mathbf{D}}_{ii} = \sum_j \tilde{\mathbf{A}}_{ij}$, and $\mathbf{W}^{(l)}$ is a layer-specific learnable weight matrix. Function $\sigma(\cdot)$ denotes a nonlinear activation function. $\mathbf{H}^{(l)} \in \mathbb{R}^{n \times d_l}$ is the matrix of d_l -dimensional hidden node representation in the l^{th} layer with $\mathbf{H}^{(0)} = \mathbf{X}$, where \mathbf{X} is the initial node feature matrix. We implement all the following models, including

- Chebyshev [56] presents a formulation of CNNs in the context of spectral graph theory, which provides the necessary mathematical background and efficient numerical schemes to design fast localized convolutional filters on graphs.
- GCN [11] proposes a well-behaved layer-wise propagation rule for neural network models which operate directly on graphs and are motivated from a first-order approximation of spectral graph convolutions.
- GAT [28] presents graph attention networks (GATs), a novel convolution-style neural networks that operate on graph-structured data, leveraging masked self-attentional layers.
- GraphSAGE [12] introduces a novel approach that allows embeddings to be efficiently generated for unseen nodes

by aggregating feature information from a node’s local neighborhood.

- APPNP [51] derives a propagation scheme from personalized PageRank by adding initial residual connection to balance locality and leverage information from a large neighborhood.
- DGI [15] introduces an approach to maximize mutual information between local representation and corresponding summaries of graphs to learn node representation in an unsupervised manner.
- GCNII [49] extends GCN to a deep model by using identity mapping and initial residual connection to resolve over-smoothing.
- MVGRL [50] proposes to use graph diffusion for data augmentation and contrasts structural views of graphs for self-supervised learning. MVGRL also maximizes local-global mutual information.
- GRAND [14] proposes to combine random propagation and consistency regularization to optimize the prediction consistency of unlabeled data across different data augmentations.
- DropEdge [54] randomly removes a certain number of edges from the input graph at each training epoch, acting like a data augmenter and also a message-passing reducer to alleviate over-fitting and over-smoothing issues.
- Graph-UNet [52] uses novel graph pooling (gPool) and unpooling (gUnpool) operations where gPool adaptively selects some nodes to form a smaller graph based on their scalar projection values on a trainable projection vector and gUnpool restores the graph.
- GDC [53] leverages generalized graph diffusion, such as heat kernel and personalized PageRank, to alleviate the problem of noisy and often arbitrarily defined edges in real graphs.
- PPRGo [58] utilizes an efficient approximation of information diffusion in GNNs based on personalized PageRank, resulting in significant speed gains.
- GraphSAINT [57] constructs minibatches by sampling the training graph and trains a full GCN on sampled subgraphs.

TABLE 9: Results of node classification on fully-supervised datasets, including full-batch and sampling-based methods. Flickr, Reddit, and ogbn-arxiv use accuracy metric, whereas PPI uses Micro-F1 metric.

	Flickr	PPI	Reddit	arxiv
GCNII	52.6 ± 0.1	96.5 ± 0.2	96.4 ± 0.0	72.5 ± 0.1
GraphSAINT	52.0 ± 0.1	99.3 ± 0.1	96.1 ± 0.0	71.5 ± 0.2
GAT	51.9 ± 0.3	97.3 ± 0.2	95.9 ± 0.1	72.3 ± 0.1
Cluster-SAGE	50.9 ± 0.1	97.9 ± 0.1	95.8 ± 0.1	69.8 ± 0.1
GCN	52.4 ± 0.1	75.7 ± 0.1	95.1 ± 0.0	71.7 ± 0.3
APPNP	52.3 ± 0.1	62.3 ± 0.1	96.2 ± 0.1	70.7 ± 0.1
PPRGo	51.1 ± 0.2	48.6 ± 0.1	94.5 ± 0.1	69.2 ± 0.1
SGC	50.2 ± 0.1	47.2 ± 0.1	94.5 ± 0.1	67.1 ± 0.0

Results and Analysis. We implement all the aforementioned GNN models and build a leaderboard for the node classification task. Table 8 and Table 9 summarize the evaluation results of all compared models in transductive and inductive datasets respectively, under the setting of node classification. We have the following observations:

- *High-order neighbors.* Plenty of studies on GNNs have focused on designing a better aggregation paradigm to incorporate neighborhood information in different distances. In citation datasets (Cora, CiteSeer, and PubMed) that are of relatively small scale, incorporating high-order information plays an important role in improving the performance of models. Most high-order models, such as GRAND, APPNP, and GDC, aim to use graph diffusion matrix $\bar{A} = \sum_{i=0}^K \alpha_i \hat{A}^i$ to collect information of distant neighbors. Methods based on diffusion are inspired by spectral graph theory and will not be troubled by the over-smoothing problem. It is light-weight and can also be applied to large-scale or unsupervised training. On the other hand, GCNII extends GCN to a deep model and uses the residual connection with identity mapping to resolve over-smoothing in GNNs. As shown in Table 8, these methods achieve remarkable results and all outperform GNNs (like GCN and GAT) that only use the immediate neighborhood information. This indicates that in these graphs, incorporating high-order information might be of great importance.
- *Dropout vs DropEdge vs DropNode.* Random propagation, such as Dropout, DropEdge, and DropNode, is critical in semi-supervised graph learning. These random methods can help avoid the overfitting problem and improve performance. In our experiments, we found that only using dropout on the same model architecture can achieve results comparable to initial models using other random propagation techniques. Theoretically, as shown in [14], random propagation in fact enforces the consistency of the classification confidence between each node and its multi-hop neighborhoods. All these random propagation methods will achieve higher gain when combined with consistency loss proposed in [14] to better leverage unlabelled data in semi-supervised settings.
- *Self-supervised learning on graphs.* Contrastive methods have been applied to graph learning and achieved remarkable results. In general, mutual information maximization and InfoNCE both have been attempted in graph representation learning. DGI and MVGRL maximize local and global mutual information. MVGRL performs better by replacing the adjacency matrix with graph diffusion matrix but is less scalable. On the contrary, GRACE, which optimizes InfoNCE, does not perform well on citation datasets with the public split. However, in our experiments, by replacing Dropout and DropEdge in GRACE with DropNode, and applying graph diffusion and mini-batch training, optimizing InfoNCE can also reach nearly 0.82 in PubMed. This indicates that graph diffusion and mini-batch training instead of full-batch might benefit graph self-supervised learning.

5.3 Graph Classification

Graph classification assigns a label to each graph and aims to map graphs into vector spaces. Graph kernels are historically dominant and employ a kernel function to measure the similarity between pairs of graphs to map graphs into vector spaces with deterministic mapping functions. But they suffer from computational bottlenecks. Recently, graph neural networks attract much attention and indeed

show promising results in this task. In the context of graph classification, GNNs often employ the readout operation to obtain a compact representation on the graph level

$$h_G = \text{READOUT}(\{h_v^{(K)} | v \in V\}). \quad (3)$$

GNNs directly apply classification based on the readout representation and thus are more efficient.

Datasets. We collect 8 popular benchmarks often used in graph classification tasks. Table 10 shows the statistics.

- **Bioinformatics datasets.** The PROTEINS dataset contains graphs of protein structures. Edges represent the interaction between sub-structures of proteins. Each graph in MUTAG, PTC, and NCI1 is a chemical compound with nodes and edges representing atoms and chemical bonds respectively. These datasets are usually have features.
- **Social networks.** IMDB-BINARY and IMDB-MULTI are movie collaboration datasets. Nodes correspond to actors/actresses and an edge means they appear in the same movie. Graphs in REDDIT-BINARY represent online discussions in reddit, where nodes correspond to users and an edge is drawn between two nodes if one responded to another’s comment. Nodes in these datasets directly use node degree as features.

Models. We implement the following graph classification models and compare their results.

- GIN [13] presents graph isomorphism network, which adjusts the weight of the central node with learning and aims to make GNN as powerful as the WeisfeilerLehman graph isomorphism test.
- DiffPool [59] proposes a differentiable pooling and generates hierarchical representation of graphs. It learns a cluster assignment matrix and can be implemented based on any GNN.
- SAGPool [60] proposes a hierarchical graph pooling method based on self-attention and considers both node features and graph topology.
- SortPool [61] rearranges nodes by sorting them according to their structural roles within the graph and then perform pooling on these nodes. Node features derived from graph convolutions are used as continuous WL colors for sorting nodes.
- PATCHY_SAN [62] orders neighbors of each node according to their graph labelings and selects the top q neighbors. The graph labelings are derived by degree, centrality and other node scores.
- DGCNN [63] builds a subgraph for each node with KNN based on node features and then applies graph convolution to the reconstructed graph.
- Infograph [64] applies contrastive learning to graph learning by maximizing the mutual information between both graph-level representation and node-level representation in an unsupervised manner.
- graph2vec [65] follows skip-gram’s training process and considers the set of all rooted subgraphs around each node as its vocabulary.
- Deep Graph Kernels (DGK) [66] learns latent representation for subgraph structures based on graph kernels in graphs with Skip-gram method.

TABLE 10: Dataset statistics for graph classification

Type	Dataset	#Graphs	#Classes	#Features	Avg. #Nodes	Avg. #Edges
Bioinformatics	MUTAG	188	2	7	17.9	19.8
	PTC	344	2	18	14.3	14.7
	PROTEINS	1,113	2	3	39.1	72.8
	NCI1	4,110	2	37	29.8	32.3
Social Networks	IMDB-B	1,000	2	-	19.8	96.5
	IMDB-M	1,500	3	-	13.0	65.9
	REDDIT-B	2,000	2	-	429.6	497.8
	COLLAB	5,000	3	-	74.5	2457.8

TABLE 11: Accuracy Results (%) of both unsupervised and supervised graph classification. \downarrow and \uparrow mean our results are lower or higher than the results in original papers. \ddagger means the experiment is not finished in 24 hours for one seed.

Algorithm	MUTAG	PTC	NCI1	PROTEINS	IMDB-B	IMDB-M	COLLAB	REDDIT-B	Reproducible
GIN [13]	92.06	67.82	81.66	75.19	76.10	51.80	79.52	83.10 \downarrow	Yes
InfoGraph [64]	88.95	60.74	76.64	73.93	74.50	51.33	79.40	76.55	Yes
graph2vec [65]	83.68	54.76 \downarrow	71.85	73.30	73.90	52.27	85.58 \uparrow	91.77	Yes
SortPool [61]	87.25	62.04	73.99 \uparrow	74.48	75.40	50.47	80.07 \uparrow	78.15	Yes
DiffPool [59]	85.18	58.00	69.09	75.30	72.50	50.50	79.27	81.20	Yes
PATCHY_SAN [62]	86.12	61.60	69.82	75.38	76.00 \uparrow	46.40	74.34	60.61	Yes
DGCNN [63]	83.33	56.72	65.96	66.75	71.60	49.20	77.45	86.20	Yes
SAGPool [60]	71.73 \downarrow	59.92	72.87	74.03	74.80	51.33	$_$ \ddagger	89.21	Yes
DGK [66]	85.58	57.28	$_$ \ddagger	72.59	55.00 \downarrow	40.40 \downarrow	$_$ \ddagger	$_$ \ddagger	Partial

As for evaluation, for supervised methods we adopt 10-fold cross-validation with 90%/10% split and repeat 10 times; for unsupervised methods, we perform the 10-fold cross-validation with LIB-SVM. Then we report the accuracy for classification performance. Table 11 reports the results of the aforementioned models on the task, including both unsupervised and supervised graph classification. We run all methods on 8 datasets and report the sorted results.

Results and Analysis. The development of GNNs for graph classification is mainly in two aspects. One line (like GIN) aims to design more powerful convolution operations to improve the expressiveness. Another line is to develop effective pooling methods to generate the graph representation.

- *Neural network vs Kernel methods.* Neural network based methods show promising results in bioinformatics datasets (MUTAG, PTC, PROTEINS, and NCI1), where nodes are with given features. But in social networks (IMDB-B, IMDB-M, COLLAB, REDDIT-B) lacking node features, methods based on graph kernels achieve really good performance and even surpass neural networks. Graph kernels are more capable of capturing structural information to discriminate non-isomorphic graphs, while GNNs are better encoders with features. Most GNNs directly perform classification based on the extracted graph representations and therefore are much more efficient than graph kernel methods.
- *Comparison between pooling methods.* Graph pooling aims to scale down the size of representations and generates graph representation from node features. Global pooling, which is used in GIN and SortPool, collects node features and applies a readout function. Hierarchical pooling, such as DiffPool and SAGPool, is proposed to capture structural information in different graph levels, including nodes and subgraphs. The experimental results indicate that, though hierarchical pooling seems more complex and intuitively would capture more information, it does

not show significant advantages over global pooling.

6 COGDL PACKAGE

In this section, we introduce the fundamental elements in CogDL including *Graph*, *Dataset*, and *Model*, as well as essential usages of CogDL.

Graph. The *Graph* is the basic data structure of CogDL to store graph data with abundant graph operations. *Graph* supports both convenient graph modification such as removing/adding edges and efficient computing such as SpMM. We also provides common graph manipulations, including adding self-loops, graph normalization, sampling neighbors, obtaining induced subgraphs, etc.

Dataset. The *dataset* component reads in data and processes it to produce tensors of appropriate types. Each dataset specifies its loss function and evaluator through function *get_loss_fn* and *get_evaluator* for training and evaluation.

Model. CogDL includes diverse graph neural networks as research baselines and for other applications. A GNN layer is implemented based on *Graph* and sparse operators. A *model* in the package consists of *model builder* and *forward propagation* functions in the PyTorch style.

6.1 Basic Usage

We provide an easy-to-use usage for experiments through *experiment* API. We can pass a dataset, a model, and hyper-parameters to the *experiment* API, which calls the low-level APIs (e.g., *train*). Producing the results with one-line command provides a convenient and efficient way to search for the best models. Furthermore, we integrate a popular library, Optuna [36], into CogDL to enable hyper-parameter search. By passing the *search_space* function that defines the search space of hyper-parameters, CogDL will start the searching and output the best results.

We put all the hyper-parameters for reproducibility in the *config* file³. Most of the parameters are obtained from hyper-parameter search in CogDL. Users can easily set *use_best_config=True* in the *experiment* API to train the model using the best parameters in the configuration file.

```
from cogdl import experiment

experiment(dataset="cora", model="gcn", hidden_size
           =32, max_epoch=200) # basic usage
```

6.2 Customized Usage

The design of CogDL makes it easy to incrementally add new or customized modules. In this part, we will show how to extend an existing graph representation algorithm in CogDL to a new scenario. We provide simple interfaces to embed a customized model/dataset into the current framework while reusing other components implemented in CogDL. The following code snippet shows how to define a customized dataset using the model in CogDL in a short clip. The new dataset will be recognized by our framework, and the *experiment* API supports the mixed use of existing and customized modules. In this way, one can easily apply any module in CogDL to a new scenario.

```
class MyDataset(NodeDataset):
    def __init__(self):
        self.path = "mydata.pt"
        super(MyDataset, self).__init__(self.path)

    def process(self):
        x, edge_index, y = load_raw_data()
        data = Graph(x=x, edge_index=edge_index, y=y)
        torch.save(data, self.path)
        return data

# Run GCN model on your own dataset
new_data = MyDataset()
experiment(dataset=new_data, model="gcn")
```

7 APPLICATIONS

In this section, we demonstrate the easy-to-use *pipeline* API and effectiveness of our toolkit for real-world applications, including paper tagging and recommendation, in AMiner⁴, a large online academic search and mining system.

Paper Tagging. Each publication in AMiner has several tags, extracted by the AMiner team using the raw texts (e.g., title and abstract) of each publication. However, publications with citation links may have similar tags, and we can utilize the citation network to improve the quality of tags. Formally, the publication tagging problem can be considered as a multi-label node classification task, where each label represents a tag. Thus, we can utilize powerful graph representation learning methods in CogDL to handle this problem. There are 4,833,171 papers in the field of computer science in the AMiner database. We conduct experiments for these papers to show how graph representation learning can

help the tagging problem. We can build an embedding generator via *generator = pipeline("generate-emb", model="prone")*. Then we can obtain the network embedding using ProNE by feeding the citation network to the generator. We choose logistic regression as the multi-label classifier. The node embeddings and raw text features can be combined to predict the tags of a given paper. The result shows that the fused features increase the recall by 12.8%, which indicates that structural information plays a vital role in tagging papers.

Recommendation. In the AMiner Subscribe page, it gives paper recommendations for AMiner users based on users' historical behaviors. CogDL supports the application of AMiner Subscribe via GNN models, since GNNs have shown great success in the recommender systems [17]. We implement several state-of-the-art GNN models for recommendation, such as LightGCN [67]. We can build a recommendation server via *recsys = pipeline("recommendation", model="lightgcn", data=data)*. We can feed a user-item interaction graph into this API and obtain the trained GNN model for serving. We can query the *recsys* with users and the system will output the recommended items.

8 CONCLUSIONS

In this paper, we introduce CogDL, an extensive toolkit for graph representation learning that provides easy-to-use APIs and efficient sparse kernel operators for researchers and developers to conduct experiments and build real-world applications. It provides standard training, evaluation, and reproducible leaderboards for most important tasks in the graph domain, including node classification, graph classification, and other graph tasks. In the future, we will explore how to support the dynamic or streaming scenario, which is more realistic in the big companies.

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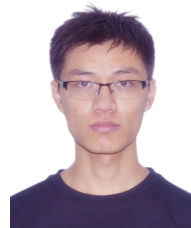
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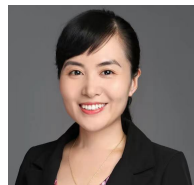
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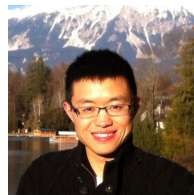


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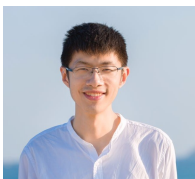


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