

CogDL: An Extensive Toolkit for Deep Learning on Graphs

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ABSTRACT

Graph representation learning aims to learn low-dimensional node embeddings for graphs. It is used in several real-world applications such as social network analysis and large-scale recommender systems. In this paper, we introduce CogDL¹, an extensive research toolkit for deep learning on graphs that allows researchers and developers to easily conduct experiments and build applications. It provides standard training and evaluation for the most important tasks in the graph domain, including node classification, link prediction, graph classification, and other graph tasks. For each task, it offers implementations of state-of-the-art models. The models in our toolkit are divided into two major parts, graph embedding methods and graph neural networks. Most of the graph embedding methods learn node-level or graph-level representations in an unsupervised way and preserves the graph properties such as structural information, while graph neural networks capture node features and work in semi-supervised or self-supervised settings. All models implemented in our toolkit can be easily reproduced for leaderboard results. Most models in CogDL are developed on top of PyTorch, and users can leverage the advantages of PyTorch to implement their own models. Furthermore, we demonstrate the effectiveness of CogDL for real-world applications in AMiner², which is a large academic database and system.

KEYWORDS

Graph neural networks; Graph representation learning; Toolkit

1 INTRODUCTION

Graph-structured data have been widely utilized in many real-world scenarios. For example, each user on Facebook can be seen as a vertex and their relations like friendship or followership can be seen as edges in the graph. We might be interested in predicting the interests of users, or whether a pair of nodes in a network should have an edge connecting them. However, traditional machine learning

algorithms cannot be directly applied to the graph-structured data. Inspired by recent trends of representation learning on computer vision and natural language processing, graph representation learning [17, 35, 45] is proposed as an efficient technique to address this issue. Graph representation aims at either learning low-dimensional continuous vectors for vertices/graphs while preserving intrinsic graph properties, or using graph encoders to an end-to-end training.

One type of network embedding is Skip-gram [30] based model, such as DeepWalk [35], LINE [45], node2vec [17], and PTE [44]. DeepWalk [35] transforms a graph structure into a uniformly sampled collection of truncated random walks and optimizes with the Skip-gram model. LINE [45] proposes loss functions to preserve both first- and second-order proximities and concatenates two learned embeddings. node2vec [17] conducts biased random walks to smoothly interpolate between breadth-first sampling (BFS) and depth-first sampling (DFS). Another type of network embedding methods is matrix factorization (MF)-based such as GraRep [5], HOPE [33], NetMF [37], and ProNE [66], which construct a proximity matrix and use MF such as singular value decomposition (SVD) [16] to obtain graph representations.

Recently, graph neural networks (GNNs) have been proposed and have achieved impressive performance in semi-supervised representation learning. Graph Convolution Networks (GCNs) [25] proposes a convolutional architecture via a localized first-order approximation of spectral graph convolutions. GraphSAGE [18] is a general inductive framework that leverages node features to generate node embeddings for previously unseen samples. Graph Attention Networks (GATs) [53] utilizes the multi-head self-attention mechanism and enables (implicitly) specifying different weights to different nodes in a neighborhood.

There are several toolkits supporting graph representation learning algorithms, such as PyTorch Geometric [13] and Deep Graph Library (DGL) [54]. PyTorch Geometric is a library for deep learning on irregularly structured input data such as graphs, point clouds, and manifolds, built upon PyTorch [34]. DGL provides flexible APIs allowing arbitrary message-passing computation over large-scale and dynamic graphs with efficient memory usage and high training speed. However, these popular graph representation learning libraries may not completely integrate various representation learning methods (e.g., Skip-gram or matrix factorization based network embedding methods). More importantly, these libraries only focus on specific downstream tasks in the graph domain (e.g., semi-supervised node classification) and do not provide sufficient reproducible evaluations of model performance.

We summarize the contributions of CogDL as follows:

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

²<https://www.aminer.cn/>

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Table 1: 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 [37]	23.73 \pm 0.22	57.42 \pm 0.56	42.47 \pm 0.35	56.72 \pm 0.14	36.27 \pm 0.17	Yes
2	ProNE [66]	24.60 \pm 0.39	56.06 \pm 0.48	41.16 \pm 0.26	56.85 \pm 0.28	36.56 \pm 0.11	Yes
3	NetSMF [36]	23.88 \pm 0.35	53.81 \pm 0.58	40.62 \pm 0.35	59.76 \pm 0.41	35.49 \pm 0.07	Yes
4	Node2vec [17]	20.67 \pm 0.54	54.59 \pm 0.51	40.16 \pm 0.29	57.36 \pm 0.39	36.13 \pm 0.13	Yes
5	LINE [45]	21.82 \pm 0.56	52.46 \pm 0.26	38.06 \pm 0.39	49.78 \pm 0.37	31.61 \pm 0.09	Yes
6	DeepWalk [35]	20.74 \pm 0.40	49.53 \pm 0.54	40.48 \pm 0.47	57.54 \pm 0.32	36.09 \pm 0.10	Yes
7	SpectralClustering [48]	22.48 \pm 0.30	49.35 \pm 0.34	41.41 \pm 0.34	43.68 \pm 0.58	33.09 \pm 0.07	Yes
8	Hope [33]	21.43 \pm 0.32	54.04 \pm 0.47	33.99 \pm 0.35	56.15 \pm 0.22	28.97 \pm 0.19	Yes
9	GraRep [5]	20.60 \pm 0.34	54.37 \pm 0.40	33.48 \pm 0.30	52.76 \pm 0.42	31.83 \pm 0.12	Yes

Table 2: Accuracy (%) reproduced by CogDL for semi-supervised and self-supervised node classification on Citation datasets. \downarrow and \uparrow mean our results are lower or higher than the result in original papers.

Rank	Method	Cora	Citeseer	Pubmed	Reproducible
1	GRAND [12]	84.8	75.1	82.4	Yes
2	GCNII [7]	85.1	71.3	80.2	Yes
3	MVGRL [20]	83.6 \downarrow	73.0	80.1	Partial
4	APPNP [26]	84.3 \uparrow	72.0	80.0	Yes
5	Graph-Unet [15]	83.3 \downarrow	71.2 \downarrow	79.0	Partial
6	GDC [27]	82.5	72.1	79.8	Yes
7	GAT [53]	82.9	71.0	78.9	Yes
8	DropEdge [38]	82.1	72.1	79.7	Yes
9	GCN [25]	82.3 \uparrow	71.4 \uparrow	79.5	Yes
10	DGI [52]	82.0	71.2	76.5	Yes
11	JK-net [58]	81.8	69.5	77.7	Yes
12	Chebyshev [8]	79.0	69.8	68.6	Yes

- **High Efficiency:** CogDL utilizes well-optimized operators to speed up training and save GPU memory of GNN models.
- **Easy-to-Use:** CogDL provides easy-to-use APIs for running experiments with the given models and datasets using hyperparameter search.
- **Extensibility:** The design of CogDL makes it easy to apply GNN models to new scenarios based on our framework.
- **Reproducibility:** CogDL provides reproducible leaderboards for state-of-the-art models on most of important tasks in the graph domain.

2 OVERVIEW

CogDL is a graph representation learning toolkit that allows researchers and developers to easily train and compare baseline or customized models for node classification, graph classification, and other important tasks in the graph domain.

Different papers may use different evaluation settings for the same graph task, making results indistinguishable. For example, as a widely used dataset, Cora [40], some papers use the “standard”

splits following Planetoid [61], while others adopt random 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 [10, 11, 23, 41]. Therefore, we propose CogDL as an open standard toolkit for graph benchmarks. The key point of CogDL is to build reproducible benchmarks for representation learning on graphs. We formalize the standard training and evaluation modules for the most important tasks in the graph domain.

The overall framework is described in Figure 1. Our framework is built on PyTorch [34], which is the most popular deep learning library. PyTorch provides an imperative and Pythonic programming style that supports code as a model, makes debugging easy. Therefore, our toolkit can leverage the advantages of PyTorch. CogDL provides implementations of several kinds of models based on Python and PyTorch, including network embedding methods such as Deepwalk, NetMF, ProNE, and GNNs such as GCN, GAT. It also supports several genres of datasets for node classification and graph classification. All the models and datasets can be utilized for experiments under different task settings in CogDL. Each task provides a standard training and evaluation pipeline for comparison.

To demonstrate the design and usage of CogDL, we will answer the following three questions, which correspond to the first three contributions summarized in Section 1:

- **Question 1:** How to efficiently train GNN models on large-scale datasets?
- **Question 2:** Which GNN algorithm does perform best on a specific dataset for a specific task?
- **Question 3:** How to easily extend an existing GNN algorithm to apply to a new scenario?

3 COGDL FRAMEWORK

In this section, we present the efficiency optimization as well as the design and usage of CogDL framework by answering the aforementioned questions.

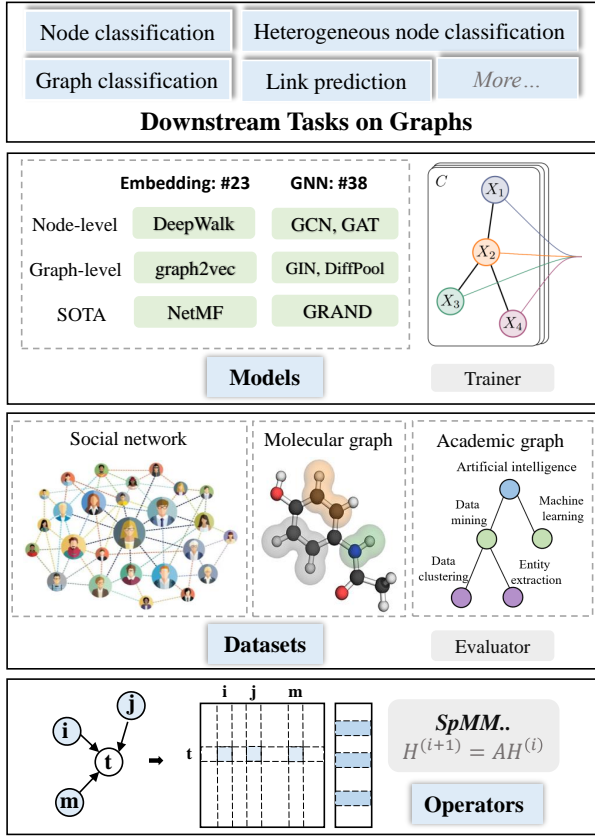


Figure 1: Overview of CogDL. CogDL mainly comprises of 3 modules: models, datasets, and downstream tasks. At the bottom, CogDL efficiently implements basic operators related to graph operations like Sparse Matrix Multiplication (SpMM). Datasets encapsulate the data structure *Data* to store graph data and specify evaluation metric by *Evaluator*. Datasets include different types of real-world graphs, including social networks, molecular graphs, academic graphs, etc. CogDL implements 23 graph embedding methods and 38 GNNs related models with specialized trainers. Based on these models and datasets, various downstream tasks are supported and are applicable to many real scenarios.

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 $A_{ij} = A_{ji}$.

Q1: Optimize the SpMM operator. We introduce an important operator used in CogDL and its corresponding optimization. The Sparse Matrix-Matrix multiplication (*SpMM*) operator is widely

used in most of GNNs. The reason is that many GNNs apply an aggregation operation for a given node from nodes of its incoming edges:

$$h_u = \text{aggregation_op}(\{h_v, \forall v \in \mathcal{N}(u)\}),$$

where $\mathcal{N}(u)$ is the set of neighbors of node u , h_u is the representation vector of node u . When the *aggregation_op* is a summation, such an operation can be described as an SpMM operator $H \leftarrow AH$, where the sparse matrix A represents the adjacency matrix of the input graph G , and each row of H represents a representation vector (e.g., h_u and h_v) of nodes. When the *aggregation_op* takes other operations, the SpMM operator can also describe the dataflow of representation vectors between nodes, while the element-wise operation varies. The *aggregation_op* can be described using a message-passing model or a Gather-Apply-Scatter (GAS) model in a general-purpose graph processing system. Many frameworks for GNNs adopt these models for SpMM implementation (e.g., *spmm* used in PyG based on the message-passing model). However, such models fail to utilize the parallelism lying in elements of a representation vector, leading to poor performance when executing SpMM operator on GPUs.

Many previous works focused on improving the performance of executing the SpMM operator on GPUs, such as ASPT [22] and GraphBlast [21]. GE-SpMM [24] is an optimized SpMM operator designed on GPUs. By avoiding redundant loading from GPU global memory and uncoalesced data access pattern, GE-SpMM improved the performance of both the SpMM operator on GPU and GNNs via SpMM. The original GE-SpMM implementation only provides support for the sparse matrix with '0-1' values, and we integrate GE-SpMM into our CogDL toolkit by extending the implementation of GE-SpMM (e.g., data loader and data format).

We compare the training and inference time of GCN models on several datasets with other popular GNN frameworks: CogDL with GE-SpMM, CogDL with *torch.spmm*, PyTorch-Geometric (PyG) v1.6.3, and Deep Graph Library (DGL) v0.5.3 with PyTorch backend. We conduct experiments using Python 3.7.5 and PyTorch v1.7.0 on a server with Intel(R) Xeon(R) CPU E5-2680 v4@2.40 GHz and Nvidia GeForce RTX 2080 Ti (11GB GPU Memory). From Table 3, CogDL with GE-SpMM achieves $3.36\times \sim 5.53\times$ speedup and $0.6\% \sim 21.7\%$ GPU memory saving compared with CogDL with *torch.spmm*. Two datasets lead to out-of-memory in PyG, and the speedup and GPU memory saving compared with DGL is $1.34\times \sim 1.73\times$.

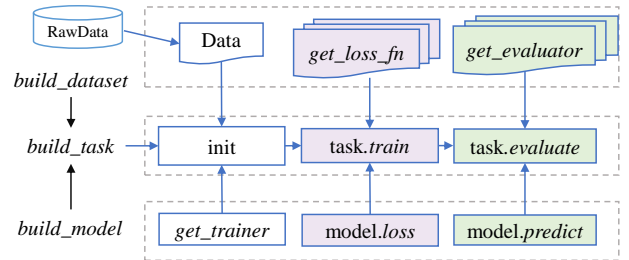


Figure 2: Architecture of CogDL.

Table 3: Epoch running time in seconds and GPU memory usage (full graph training). One epoch includes one training with back-propagation and one inference. The model includes 2 GCN layers and hidden-size is set to 128. OOM means out-of-memory.

Dataset	CogDL with GE-SpMM		CogDL with torch.spmmm		PyTorch Geometric (PyG)		Deep Graph Library (DGL)	
	Time	Memory	Time	Memory	Time	Memory	Time	Memory
Flickr	0.011	1.47G	0.037	1.53G	0.023	2.38G	0.019	1.70G
Reddit	0.119	3.81G	0.658	4.87G	/	OOM	0.159	4.34G
Yelp	0.145	7.13G	0.596	7.17G	/	OOM	0.220	8.99G

Q2: Easy-to-use design and usage. We introduce the design of CogDL and show how to use CogDL to find the best algorithm. Based on the backend and bottom operators, CogDL comprises three modules: *Datasets*, *Models*, and *Tasks*. The architecture of CogDL is illustrated in Figure 2. The three components work together to serve downstream applications and are defined independently.

Task. The *task* module puts the model and dataset together. The model and dataset are specified in *args* and built in the *task* through APIs in the package. *task.train()* runs the training and evaluation of models and datasets specified in *args* and returns the performance. After the training, parameters of model and node/graph representations will be saved for further usage.

Dataset. The *dataset* component reads in data and processes it to produce tensors of appropriate types. Each graph is stored as *Data*, the basic data structure supporting basic graph operations like *sub-graph* and *random walk*. Loss function and evaluator are specified in *Dataset* and exposed through *get_loss_fn* and *get_evaluator* for later usage on training and evaluation. The package provides many real-world datasets and interfaces for users to define customized datasets with *register_dataset*.

Model. A *model* in the package comprises *forward propagation* and *loss computation*. The loss can consist of auxiliary parts for training. In addition, the library supports specifying a customized *trainer* for a model through *get_trainer*. Details of the trainer can be found in Appendix A.2.4. Similar to *Dataset*, the model should be *registered* to make it known to the framework.

We provide a more easy-to-use usage for experiments through *experiment* API. A quickstart example is listed below.

```
1 from cogdl import experiment
2
3 # basic usage
4 experiment(task="node_classification", dataset="cora", model="gcn",
5           hidden_size=32, max_epoch=200)
6
7 # basic usage for hyper-parameter search
8 experiment(task="node_classification", dataset="cora", model="gcn",
9           func_search=func_search)
```

We can pass a specific task, dataset, model with hyper-parameters to the *experiment* API, which calls the low-level APIs (e.g., *build_task* and *task.train*). We also integrate a popular library, *optuna* [1] to enable hyper-parameter search in CogDL by passing *func_search* function which defines the search space of hyper-parameters.

We put all the hyper-parameters for reproducibility in the *config* file³. Users can easily set *use_best_config=True* in the *experiment*

API to train the model using the best parameters in the configuration file.

Q3: Define new modules. 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. Quickly applying existing GNN algorithms to new scenarios will help leverage existing methods to benefit academia and industry. We provide very simple interfaces to make it convenient to embed a customized model/dataset/task into the current framework. Therefore, in addition to the above tasks, CogDL also provides the implementations of abundant tasks in the graph domain: heterogeneous node classification, multiplex link prediction, knowledge graph completion, etc.

The following code snippet shows how to define a new task *community_detection* with existing or customized dataset in a short clip. The new task and dataset will be collected by our framework when *@register* is called, and the *experiment* supports the mixed-use of an existing and customized modules. In this way, one can easily apply any module in CogDL to a new scenario.

```
1 @register_task("community_detection")
2 class CommunityDetection(BaseTask):
3     def __init__(self, args):
4         dataset = build_dataset(args)[0]
5         self.data = dataset.data
6         self.evaluator = dataset.get_evaluator()
7         self.model = build_model(args)
8
9     def train(self):
10        for i in range(self.max_epoch):
11            self.model.loss(self.data).backward()
12            self.optimizer.step()
13        return self.evaluator(self.model.predict(self.data), self.data.y)
14
15 experiment(task="community_detection", dataset="dblp", model="gcn")
16
17 @register_dataset("new_data")
18 class CustomizedDataset(BaseDataset):
19     def __init__(self):
20         self._process()
21         self.data = torch.load("mydata.pt")
22
23     def process(self):
24         x, edge_index, y = load_raw_data()
25         data = Data(x=x, edge_index=edge_index, y=y)
26         torch.save(data, "mydata.pt")
27
28 experiment(task="community_detection", dataset="new_data", model="gcn")
```

³<https://github.com/THUDM/cogdl/blob/master/cogdl/configs.py>

4 GRAPH BENCHMARKS

In this section, with CogDL, we provide several downstream tasks including node classification, link prediction, 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.

4.1 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 4 shows the statistics of these datasets.

- BlogCatalog [64] is a social blogger network, where nodes and edges stand for bloggers and their social relationships, respectively. Bloggers' interests are used as labels.
- Wikipedia⁴ 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 [49].
- PPI [4] is a subgraph of the PPI network for Homo Sapiens. Node labels are extracted from hallmark gene sets and represent biological states.
- DBLP [46] is an academic citation network where authors are treated as nodes and their dominant conferences as labels.
- Flickr [47] 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, including DeepWalk [35], LINE [45], and node2vec [17]. The other is matrix factorization based models, including SpectralClustering [48], GraRep [5], NetMF [37], ProNE [66], NetSMF [36].

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. Thus given a graph, any kind of proximity can be exploited by network embedding models, such as Adjacency proximity, Adamic-Adar proximity, Katz proximity, Jaccard's coefficient proximity, SimRank proximity, etc. Actually, NetMF [37] 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 1 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 (SG) 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 SG 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 $\sum_{i=0}^k \alpha_i A^i$ rather than adjacency matrix 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.

4.2 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 transductive and inductive settings.

- Transductive datasets include three citation networks, Citeseer, Cora, and Pubmed [40]. 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 A . Each document has a class label. For training, we only use 20 labels per class, but all feature vectors.
- Inductive datasets include social networks (Reddit, Yelp, and Flickr) and bioinformatics (PPI) from GraphSAINT [65]. 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.

Models. GCNs [25] extend the convolution operation into graph-structured data by applying layer-wise propagation rule:

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

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

⁴<http://www.mattmahoney.net/dc/text.html>

Table 4: Dataset statistics for node classification (“m” stands for multi-label classification)

Setting	Dataset	#Nodes	#Edges	#Features	#Classes	# Train / Val / Test
Semi-supervised (Transductive)	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
Supervised (Inductive)	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
Unsupervised	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

l^{th} layer with $\mathbf{H}^{(0)} = \mathbf{X}$, where \mathbf{X} is the initial node feature matrix. Graph diffusion based GNNs aggregates information not only from the first-hop neighbors but from a larger neighborhood. A general graph diffusion matrix is defined as

$$\tilde{\mathbf{A}} = \sum_{i=0}^{K-1} \alpha_i \hat{\mathbf{A}}^i.$$

Graph diffusion convolution network (GDC) [27] just replaces adjacency matrix $\hat{\mathbf{A}}$ with $\tilde{\mathbf{A}}$. Besides GCN and GDC, we also implement all the following models, including ChebyNet [8], GAT [53], GraphSAGE [18], APPNP [26], DGI [52], GCNII [7], MVGRL [20], GRAND [12], DropEdge [38], Graph-Unet [15], PPRGo [2], GraphSAINT [65]. Details of these models can be referred to Appendix A.1.

Table 5: Micro-F1 (%) for node classification on inductive datasets, including full-batch and sampling-based methods. “-” means that the performance of the model on these datasets is not reported in the paper.

	Flickr	PPI	Reddit	Reproducible
GCN	52.4 ± 0.1	75.7 ± 0.1	95.1 ± 0.0	-
APPNP	52.3 ± 0.1	62.3 ± 0.1	96.2 ± 0.1	-
GraphSAINT	52.0 ± 0.1	96.6 ± 0.1	96.1 ± 0.0	Partial
GCNII	52.6 ± 0.1	96.5 ± 0.2	96.4 ± 0.0	Partial
PPRGo	51.1 ± 0.2	48.6 ± 0.1	94.5 ± 0.1	-

Results and Analysis. We implement all the aforementioned GNN models and build a leaderboard for the node classification task. Table 2 and Table 5 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 $\tilde{\mathbf{A}} = \sum_{i=0}^{K-1} \alpha_i \hat{\mathbf{A}}^i$ 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 2, 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 [12], 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 [12] 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, doesn’t perform well on citation datasets with the public split. However, in our experiments, by replacing drop-feature and drop-edge 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.

4.3 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 pooling and readout operations to obtain a compact representation on the graph level

$$\mathbf{h}_G = \text{READOUT}(\{\mathbf{h}_v^{(l)} | v \in G\}).$$

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 6 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 [57], DiffPool [62], SAGPool [28], SortPool [67], DGCNN [56] and Infograph [42] are based on GNNs. PATCHY_SAN [32] is inspired by convolutional neural networks. Deep graph kernels (DGK) [59] and graph2vec [31] use graph kernels.

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 7 reports the results of the aforementioned models on the task, including both unsupervised and supervised graph classification. We run all algorithms in 8 datasets and report the sorted experimental 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.

4.4 Other Graph Tasks

CogDL also provides other important tasks in the graph domain, including heterogeneous node classification, link prediction, multiplex link prediction, and knowledge graph completion.

Heterogeneous Node Classification. This task is built for heterogeneous GNNs conducted on heterogeneous graphs. For heterogeneous node classification, we use macro-F1 to evaluate the performance of all heterogeneous models under the setting of Graph Transformer Networks (GTN) [63]. The heterogeneous datasets include DBLP, ACM, and IMDB. We implement and compare the heterogeneous models, including GTN [63], HAN [55], PTE [44], metapath2vec [9], hin2vec [14].

Link Prediction. Liben-Nowell and Kleinberg [29] studied the underlying social-network evolution and proposed a basic computational problem named link prediction: Given a snapshot of a social network at time t , it seeks to accurately predict the edges that will be added to the network during the interval from time t to a given future time. In CogDL, we remove 15 percents of edges for each dataset and adopt ROC AUC [19] as the evaluation metric, which is the area under the receiver operating characteristic curve.

Multiplex Link Prediction. GATNE [6] formalizes the problem of embedding learning for the Attributed Multiplex Heterogeneous Network and proposes a unified framework to solve it with both transductive and inductive settings. We follow the setting of GATNE [6] to build the multiplex heterogeneous link prediction task. In CogDL, for those methods that only deal with homogeneous networks, we feed separate graphs with different edge types to them and obtain different node representations for each separate graph. We also adopt ROC AUC as the evaluation metric.

Knowledge Graph Completion. This task aims to predict missing links in a knowledge graph through knowledge graph embedding. In CogDL, we implement two families of knowledge graph embedding algorithms: triplet-based knowledge graph embedding and knowledge-based GNNs. The former includes TransE [3], DistMult [60], ComplEx [50], and RotatE [43]; the latter includes RGCN [39]

Table 6: 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 7: Results (Accuracy) of both unsupervised and supervised graph classification. ↓ and ↑ mean our results are lower or higher than the results in original papers.

Algorithm	MUTAG	PTC	NCI1	PROTEINS	IMDB-B	IMDB-M	COLLAB	REDDIT-B	Reproducible
GIN [57]	92.06	67.82	81.66	75.19	76.10	51.80	79.52	83.10 ↓	Yes
InfoGraph [42]	88.95	60.74	76.64	73.93	74.50	51.33	79.40	76.55	Yes
DiffPool [62]	85.18	58.00	69.09	75.30	72.50	50.50	79.27	81.20	Yes
SortPool [67]	87.25	62.04	73.99 ↑	74.48	75.40	50.47	80.07 ↑	78.15	Yes
graph2vec [31]	83.68	54.76 ↓	71.85	73.30	73.90	52.27	85.58 ↑	91.77	Yes
PATCHY_SAN [32]	86.12	61.60	69.82	75.38	76.00 ↑	46.40	74.34	60.61	Yes
DGCNN [56]	83.33	56.72	65.96	66.75	71.60	49.20	77.45	86.20	Yes
SAGPool [28]	71.73 ↓	59.92	72.87	74.03	74.80	51.33	/	89.21	Yes
DGK [59]	85.58	57.28	/	72.59	55.00 ↓	40.40 ↓	/	/	Partial

and CompGCN [51]. We evaluate all implemented algorithms with standard benchmarks including FB15k-237, WN18 and WN18RR and use Mean Reciprocal Rank (MRR) as the evaluation metric.

5 APPLICATIONS

In this section, we demonstrate the effectiveness of our toolkit for a real-world application in AMiner, a large academic database and system. 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 train a network embedding using ProNE on the citation network, and use logistic regression as the multi-label classifier. And then we combine the embedding and raw text features 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.

In addition, CogDL has gained users from academia like Carnegie Mellon University, Shanghai Jiaotong University, and Kungliga Tekniska högskolan for study or research in graph computing,

graph analysis, etc. Our package is also forked by developers in the industry like Microsoft and Tencent to help their work.

6 CONCLUSIONS

In this paper, we introduce CogDL, an extensive research toolkit for graph representation learning that allows researchers and developers to easily conduct experiments and reproduce state-of-the-art results. It provides standard training and evaluation for most of important tasks in the graph domain, including node classification, link prediction, graph classification, and other graph tasks. We run experiments on all models implemented in our toolkit and build reproducible leaderboards for them.

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A APPENDIX

A.1 Models

In this section, we list the details of all models implemented in CogDL. We summarize these models in Table 8.

Unsupervised Node Classification

- SpectralClustering [48] generates node representations from the d -smallest eigenvectors of the normalized graph Laplacian.
- DeepWalk [35] transforms a graph structure into linear sequences by truncating random walks and processing the sequences using Skip-gram with hierarchical softmax.
- LINE [45] defines loss functions to preserve first-order or second-order proximity separately and concatenates two representations together.
- node2vec [17] 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 [5] decomposes k -step probability transition matrix to train the node embedding, then concatenate all k -step representations.
- HOPE [33] approximates high-order proximity based on factorizing the Katz matrix.
- NetMF [37] shows that Skip-gram models with negative sampling like Deepwalk, LINE can be unified into the matrix factorization framework with closed forms.
- ProNE [66] firstly transforms the graph representation learning into decomposition of a sparse matrix, and further improves the performance through spectral propagation technology.
- NetSMF [36] addresses the efficiency and scalability challenges faced by the NetMF model via achieving a sparsification of the (dense) NetMF matrix.

Semi-supervised Node Classification

- Chebyshev [8] 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 [25] 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 [53] presents graph attention networks (GATs), a novel convolution-style neural networks that operate on graph-structured data, leveraging masked self-attentional layers.
- GraphSAGE [18] 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 [26] derives a propagation scheme from personalized PageRank by adding initial residual connection to balance locality and leverage information from a large neighborhood.
- DGI [52] introduces an approach to maximize mutual information between local representation and corresponding summaries of graphs to learn node representation in an unsupervised manner.

- GCNII [7] extends GCN to a deep model by using identity mapping and initial residual connection to resolve over-smoothing.
- MVGRL [20] 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 [12] proposes to combine random propagation and consistency regularization to optimize the prediction consistency of unlabeled data across different data augmentations.
- DropEdge [38] randomly removes a certain number of edges from the input graph at each training epoch, acting like a data augmentor and also a message-passing reducer to alleviate over-fitting and over-smoothing issues.
- Graph-Unet [15] 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 [27] 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 [2] utilizes an efficient approximation of information diffusion in GNNs based on personalized PageRank, resulting in significant speed gains.
- GraphSAINT [65] constructs minibatches by sampling the training graph and trains a full GCN on sampled subgraphs.

Graph Classification

- GIN [57] 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 [62] 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 [28] proposes a hierarchical graph pooling method based on self-attention and considers both node features and graph topology.
- SortPool [67] 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 [32] 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 [56] builds a subgraph for each node with KNN based on node features and then applies graph convolution to the reconstructed graph.
- Infograph [42] 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 [31] follows skip-gram’s training process and considers the set of all rooted subgraphs around each node as its vocabulary.
- Deep Graph Kernels (DGK) [59] learns latent representation for subgraph structures based on graph kernels in graphs with Skip-gram method.

Table 8: Summarization of implemented models for node classification and graph classification tasks.

Task	Characteristics		Models
Node Classification (Unsupervised)	Matrix Factorization		SpectralClustering [48]
		With high-order neighborhood	NetMF [37], ProNE [66], NetSMF [36], HOPE [33], GraRep [5]
	Skip-gram		LINE [45]
		With high-order neighborhood	DeepWalk [35], Node2vec [17]
Node Classification (with GNN)	Semi-supervised		GCN [25], GAT [53], JK-Net [58], ChebyNet [8], GCNII [7]
		With random propagation	DropEdge [38], Graph-Unet [15], GraphSAINT [65], GRAND [12]
		With diffusion	GDC [27], APPNP [26], GRAND [12], PPRGo [2]
	Self-supervised	Contrastive methods	MVGRL [20], DGI [52]
Graph Classification	Supervised	CNN method	PATCHY_SAN [32]
		Global pooling	GIN [57], SortPool [67], DGCNN [56]
		Hierarchical pooling	DiffPool [62], SAGPool [28]
	Unsupervised	Kernel methods	DGK [59], graph2vec [31]
		GNN method	Infograph [42]

A.2 CogDL Package

In this section, we introduce the key components of the CogDL package, including *Task*, *Dataset*, *Model*, and *Trainer*.

A.2.1 Task. The model and dataset are specified in *args* and built in *task*. *train* is the only exposed API for a task and integrates the training and evaluation. Flexibly, loss optimization can also be implemented in *train* for task-specific targets. *task.train()* runs the training and evaluation of models and datasets specified in *args* and returns the performance. After the training, parameters of model and node/graph representations will be saved for further plan.

A.2.2 Dataset. The *Dataset* component reads in data from a persistent storage and processes the graph to produce tensors of the appropriate types. The library provides two ways to fit a customized dataset. One way is to convert raw data files into the required format in CogDL and specify the argument *data_path*, then CogDL will read and process the data with pre-defined functions. In addition, the library allows developers to define customized dataset class. The loss function and metric evaluator should be set. Finally the customized dataset must be "registered" to CogDL.

```

1 @register_dataset("my_dataset")
2 class MyDataset(BaseDataset):
3     ...
4     def get_evaluator(self):
5         return accuracy
6     def get_loss_fn(self):
7         return cross_entropy_loss

```

A.2.3 Model. A *Model* in the library comprises of *model builder*, *forward propagation* and *loss calculation*. APIs described below are implemented in each model to provide a unified paradigm for usage. *add_args* and *build_model_from_args* are used to build up a model with model-specific hyper-parameters. *loss* takes in the data, calls the core *forward* function and returns the loss in one propagation. The loss can consist of auxiliary parts for training,

like regularization loss. In addition, the library supports specifies a customized trainer for a model. Each model should be *registered* in the library. The code snippet below shows a simple implementation of a GNN model.

```

1 @register("sslgnn")
2 class SSLGNNModel(nn.Module):
3     def add_args(parser):
4         parser.add_argument("--wd", type=float,)
5
6     def loss(self, data):
7         pred = self.forward(x, edge_index)
8         return loss_fn(pred, labels) + self.wd * norm(pred)/2
9
10    def get_trainer():
11        return SelfSupervisedTrainer

```

A.2.4 Trainer. *Trainer* is a supplement component for *Task*. The training or evaluation of some models are special and incompatible with the general paradigm in CogDL. In such cases, a custom-built trainer can be constructed in CogDL and specified in the model with *get_trainer*, as show in Section A.2.3. *trainer.fit*, which is similar to the function *task.train* and covers training and evaluation, takes model and dataset as input and returns the performance. *Trainer* is used only when it is specified in a model, and then the trainer will take over the process. The code snippet below together with the snippet in Section A.2.3 shows how a trainer is specified and used.

```

1 class SelfSupervisedTrainer(BaseTrainer):
2     def fit(self, model, dataset):
3         """Training Process."""
4
5 class NodeClassification(BaseTask):
6     def __init__(self, args):
7         ...
8         self.trainer = self.model.get_trainer()
9
10    def train(self):
11        if self.trainer is not None:
12            result = self.trainer.fit(self.model, self.dataset)

```