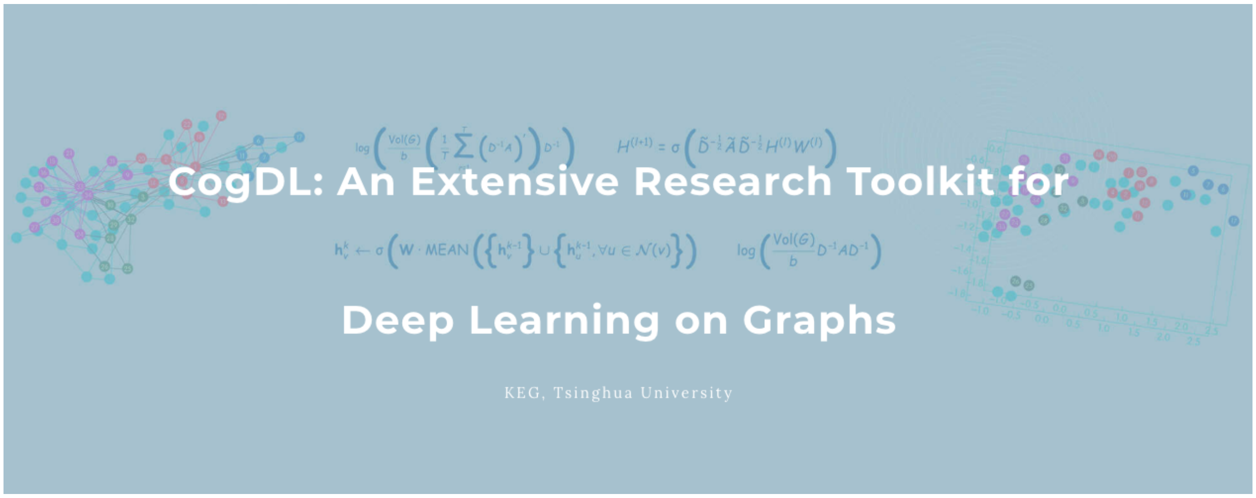
CogDL Documentation

Release 0.5.3

KEG

Jun 01, 2022

GET STARTED



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.

We summarize the contributions of CogDL as follows:

- **Efficiency**: CogDL utilizes well-optimized operators to speed up training and save GPU memory of GNN models.
- **Ease of Use**: CogDL provides easy-to-use APIs for running experiments with the given models and datasets using hyper-parameter search.
- **Extensibility**: The design of CogDL makes it easy to apply GNN models to new scenarios based on our framework.

CHAPTER

ONE

NEWS

- The new **v0.5.3 release** supports mixed-precision training by setting textit{fp16=True} and provides a basic [example](https://github.com/THUDM/cogdl/blob/master/examples/jittor/gcn.py) written by [Jittor](https://github.com/Jittor/jittor). It also updates the tutorial in the document, fixes downloading links of some datasets, and fixes potential bugs of operators.
- The new **v0.5.2 release** adds a GNN example for ogbn-products and updates geom datasets. It also fixes some potential bugs including setting devices, using cpu for inference, etc.
- The new **v0.5.1 release** adds fast operators including SpMM (cpu version) and scatter_max (cuda version). It also adds lots of datasets for node classification.
- The new **v0.5.0 release** designs and implements a unified training loop for GNN. It introduces *DataWrapper* to help prepare the training/validation/test data and *ModelWrapper* to define the training/validation/test steps.
- The new **v0.4.1 release** adds the implementation of Deep GNNs and the recommendation task. It also supports new pipelines for generating embeddings and recommendation. Welcome to join our tutorial on KDD 2021 at 10:30 am - 12:00 am, Aug. 14th (Singapore Time). More details can be found in https://kdd2021graph.github.io/.
- The new **v0.4.0 release** refactors the data storage (from `Data` to `Graph`) and provides more fast operators to speed up GNN training. It also includes many self-supervised learning methods on graphs. BTW, we are glad to announce that we will give a tutorial on KDD 2021 in August. Please see this link for more details.
- The new **v0.3.0 release** provides a fast spmm operator to speed up GNN training. We also release the first version of CogDL paper in arXiv. You can join our slack for discussion.
- The new **v0.2.0 release** includes easy-to-use `experiment` and `pipeline` APIs for all experiments and applications. The `experiment` API supports automl features of searching hyper-parameters. This release also provides `OAGBert` API for model inference (`OAGBert` is trained on large-scale academic corpus by our lab). Some features and models are added by the open source community (thanks to all the contributors).
- The new **v0.1.2 release** includes a pre-training task, many examples, OGB datasets, some knowledge graph embedding methods, and some graph neural network models. The coverage of CogDL is increased to 80%. Some new APIs, such as `Trainer` and `Sampler`, are developed and being tested.
- The new **v0.1.1 release** includes the knowledge link prediction task, many state-of-the-art models, and `optuna` support. We also have a Chinese WeChat post about the CogDL release.

CHAPTER

TWO

CITING COGDL

Please cite our paper if you find our code or results useful for your research:

```
@article{cen2021cogdl,
   title={CogDL: A Toolkit for Deep Learning on Graphs},
   author={Yukuo Cen and Zhenyu Hou and Yan Wang and Qibin Chen and Yizhen Luo and␣
↪Zhongming Yu and Hengrui Zhang and Xingcheng Yao and Aohan Zeng and Shiguang Guo and␣
↪Yuxiao Dong and Yang Yang and Peng Zhang and Guohao Dai and Yu Wang and Chang Zhou and␣
↪Hongxia Yang and Jie Tang},
   journal={arXiv preprint arXiv:2103.00959},
   year={2021}
}
```

2.1 Install

- Python version >= 3.7
- PyTorch version >= 1.7.1

Please follow the instructions here to install PyTorch (https://github.com/pytorch/pytorch#installation).

When PyTorch has been installed, cogdl can be installed using pip as follows:

```
pip install cogdl
```

Install from source via:

```
pip install git+https://github.com/thudm/cogdl.git
```

Or clone the repository and install with the following commands:

```
git clone git@github.com:THUDM/cogdl.git
cd cogdl
pip install -e .
```

If you want to use the modules from PyTorch Geometric (PyG), you can follow the instructions to install PyTorch Geometric (https://github.com/rusty1s/pytorch_geometric/#installation).

2.2 Quick Start

2.2.1 API Usage

You can run all kinds of experiments through CogDL APIs, especially `experiment()`. You can also use your own datasets and models for experiments. A quickstart example can be found in the quick_start.py. More examples are provided in the examples/.

```python
from cogdl import experiment

# basic usage
experiment(dataset="cora", model="gcn")

# set other hyper-parameters
experiment(dataset="cora", model="gcn", hidden_size=32, epochs=200)

# run over multiple models on different seeds
experiment(dataset="cora", model=["gcn", "gat"], seed=[1, 2])

# automl usage
def search_space(trial):
    return {
        "lr": trial.suggest_categorical("lr", [1e-3, 5e-3, 1e-2]),
        "hidden_size": trial.suggest_categorical("hidden_size", [32, 64, 128]),
        "dropout": trial.suggest_uniform("dropout", 0.5, 0.8),
    }

experiment(dataset="cora", model="gcn", seed=[1, 2], search_space=search_space)
```

2.2.2 Command-Line Usage

You can also use `python scripts/train.py --dataset example_dataset --model example_model` to run example_model on example_data.

- `--dataset`, dataset name to run, can be a list of datasets with space like `cora citeseer`. Supported datasets include `cora`, `citeseer`, `pumbed`, `ppi`, `flickr`. More datasets can be found in the cogdl/datasets.
- `--model`, model name to run, can be a list of models like `gcn gat`. Supported models include `gcn`, `gat`, `graphsage`. More models can be found in the cogdl/models.

For example, if you want to run GCN and GAT on the Cora dataset, with 5 different seeds:

`` `bash python scripts/train.py --dataset cora --model gcn gat --seed 0 1 2 3 4 ` ``

Expected output:

Variant	test_acc	val_acc
('cora', 'gcn')	0.8050±0.0047	0.7940±0.0063
('cora', 'gat')	0.8234±0.0042	0.8088±0.0016

If you want to run parallel experiments on your server with multiple GPUs on multiple models/datasets:

```
python scripts/train.py --dataset cora citeseer --model gcn gat --devices 0 1 --seed 0 1␣
↪2 3 4
```

Expected output:

Variant	test_acc	val_acc
('cora', 'gcn')	0.8050±0.0047	0.7940±0.0063
('cora', 'gat')	0.8234±0.0042	0.8088±0.0016
('citeseer', 'gcn')	0.6938±0.0133	0.7108±0.0148
('citeseer', 'gat')	0.7098±0.0053	0.7244±0.0039

2.3 Introduction to Graphs

2.3.1 Real-world graphs

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 might have an edge connecting them.

2.3.2 How to represent a graph in CogDL

A graph is used to store information of structured data. CogDL represents a graph with a `cogdl.data.Graph` object. Briefly, a `Graph` holds the following attributes:

- `x`: Node feature matrix with shape `[num_nodes, num_features]`, *torch.Tensor*
- `edge_index`: COO format sparse matrix, *Tuple*
- `edge_weight`: Edge weight with shape `[num_edges,]`, *torch.Tensor*
- `edge_attr`: Edge attribute matrix with shape `[num_edges, num_attr]`
- `y`: Target labels of each node, with shape `[num_nodes,]` for single label case and *[num_nodes, num_labels]* for mult-label case
- `row_indptr`: Row index pointer for CSR sparse matrix, *torch.Tensor*.
- `col_indices`: Column indices for CSR sparse matrix, *torch.Tensor*.
- `num_nodes`: The number of nodes in graph.
- `num_edges`: The number of edges in graph.

The above are the basic attributes but are not necessary. You may define a graph with *g = Graph(edge_index=edges)* and omit the others. Besides, `Graph` is not restricted to these attributes and other self-defined attributes, e.g., *graph.mask = mask*, are also supported.

`Graph` stores sparse matrix with COO or CSR format. COO format is easier to add or remove edges, e.x. *add_self_loops*, and CSR is stored for fast message-passing. `Graph` automatically convert between two formats and you can use both on demands without worrying. You can create a Graph with edges or assign edges to a created graph. *edge_weight* will be automatically initialized as all ones, and you can modify it to fit your need.

```
import torch
from cogdl.data import Graph
edges = torch.tensor([[0,1],[1,3],[2,1],[4,2],[0,3]]).t()
g = Graph()
g.edge_index = edges
```

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```
g = Graph(edge_index=edges) # equivalent to that above
print(g.edge_weight)
>> tensor([1., 1., 1., 1., 1.])
g.num_nodes
>> 5
g.num_edges
>> 5
g.edge_weight = torch.rand(5)
print(g.edge_weight)
>> tensor([0.8399, 0.6341, 0.3028, 0.0602, 0.7190])
```

We also implement commonly used operations in `Graph`:

- `add_self_loops`: add self loops for nodes in graph,

$$\hat{A} = A + I$$

- `add_remaining_self_loops`: add self-loops for nodes without it.
- `sym_norm`: symmetric normalization of edge_weight used *GCN*:

$$\hat{A} = D^{-1/2}AD^{-1/2}$$

- `row_norm`: row-wise normalization of edge_weight:

$$\hat{A} = D^{-1}A$$

- `degrees`: get degrees for each node. For directed graph, this function returns in-degrees of each node.

```
import torch
from cogdl.data import Graph
edge_index = torch.tensor([[0,1],[1,3],[2,1],[4,2],[0,3]]).t()
g = Graph(edge_index=edge_index)
>> Graph(edge_index=[2, 5])
g.add_remaining_self_loops()
>> Graph(edge_index=[2, 10], edge_weight=[10])
>> print(edge_weight) # tensor([1., 1., ..., 1.])
g.row_norm()
>> print(edge_weight) # tensor([0.3333, ..., 0.50])
```

- `subgraph`: get a subgraph containing given nodes and edges between them.
- `edge_subgraph`: get a subgraph containing given edges and corresponding nodes.
- `sample_adj`: sample a fixed number of neighbors for each given node.

```
from cogdl.datasets import build_dataset_from_name
g = build_dataset_from_name("cora")[0]
g.num_nodes
>> 2707
g.num_edges
>> 10184
# Get a subgraph contaning nodes [0, .., 99]
sub_g = g.subgraph(torch.arange(100))
>> Graph(x=[100, 1433], edge_index=[2, 18], y=[100])
# Sample 3 neighbors for each nodes in [0, .., 99]
```

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```
nodes, adj_g = g.sample_adj(torch.arange(100), size=3)
>> Graph(edge_index=[2, 300]) # adj_g
```

- `train/eval`: In inductive settings, some nodes and edges are unseen during training, `train/eval` provides access to switching backend graph for training/evaluation. In transductive setting, you may ignore this.

```
# train_step
model.train()
graph.train()

# inference_step
model.eval()
graph.eval()
```

2.3.3 How to construct mini-batch graphs

In node classification, all operations are in one single graph. But in tasks like graph classification, we need to deal with many graphs with mini-batch. Datasets for graph classification contains graphs which can be accessed with index, e.x. `data[2]`. To support mini-batch training/inference, CogDL combines graphs in a batch into one whole graph, where adjacency matrices form sparse block diagnal matrices and others(node features, labels) are concatenated in node dimension. `cogdl.data.Dataloader` handles the process.

```
from cogdl.data import DataLoader
from cogdl.datasets import build_dataset_from_name

dataset = build_dataset_from_name("mutag")
>> MUTAGDataset(188)
dataswet[0]
>> Graph(x=[17, 7], y=[1], edge_index=[2, 38])
loader = DataLoader(dataset, batch_size=8)
for batch in loader:
    model(batch)
>> Batch(x=[154, 7], y=[8], batch=[154], edge_index=[2, 338])
```

`batch` is an additional attributes that indicate the respective graph the node belongs to. It is mainly used to do global pooling, or called *readout* to generate graph-level representation. Concretely, `batch` is a tensor like:

$$batch = [0, .., 0, 1, ..., 1, N - 1, ..., N - 1]$$

The following code snippet shows how to do global pooling to sum over features of nodes in each graph:

```
def batch_sum_pooling(x, batch):
    batch_size = int(torch.max(batch.cpu())) + 1
    res = torch.zeros(batch_size, x.size(1)).to(x.device)
    out = res.scatter_add_(
        dim=0,
        index=batch.unsqueeze(-1).expand_as(x),
        src=x
       )
    return out
```

2.3.4 How to edit the graph?

Changes can be applied to edges in some settings. In such cases, we need to *generate* a graph for calculation while keep the original graph. CogDL provides *graph.local_graph* to set up a local scape and any out-of-place operation will not reflect to the original graph. However, in-place operation will affect the original graph.

```
graph = build_dataset_from_name("cora")[0]
graph.num_edges
>> 10184
with graph.local_graph():
    mask = torch.arange(100)
    row, col = graph.edge_index
    graph.edge_index = (row[mask], col[mask])
    graph.num_edges
    >> 100
graph.num_edges
>> 10184

graph.edge_weight
>> tensor([1.,...,1.])
with graph.local_graph():
    graph.edge_weight += 1
graph.edge_weight
>> tensor([2.,...,2.])
```

2.3.5 Common graph datasets

CogDL provides a bunch of commonly used datasets for graph tasks like node classification, graph classification and others. You can access them conveniently shown as follows. Statistics of datasets are on this page .

```
from cogdl.datasets import build_dataset_from_name
dataset = build_dataset_from_name("cora")

from cogdl.datasets import build_dataset
dataset = build_dataset(args) # if args.dataet = "cora"
```

For all datasets for node classification, we use *train_mask*, *val_mask*, *test_mask* to denote train/validation/test split for nodes.

2.4 Model Training

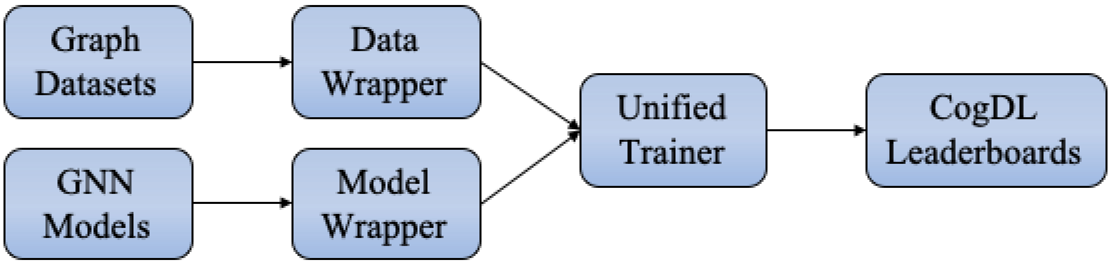
2.4.1 Introduction to graph representation learning

Inspired by recent trends of representation learning on computer vision and natural language processing, graph representation learning 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.

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

2.4.2 Unified Trainer

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

Paper	Model	Model Wrapper	Data Wrapper
GCN	GCN	supervised	full-graph
GAT	GAT	supervised	full-graph
GraphSAGE	SAGE	sage_mw	neighbor sampling
Cluster-GCN	GCN	supervised	graph clustering
DGI	GCN	dgi_mw	full-graph

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 textit{trainer = Trainer(epochs,…)} and textit{trainer.run(…)}. Moreover, based on the unified trainer, CogDL provides native support for many useful features, including hyperparameter optimization, efficient training techniques, and experiment management without any modification to the model implementation.

2.4.3 Experiment API

CogDL provides a more easy-to-use API upon *Trainer*, i.e., *experiment*. We take node classification as an example and show how to use CogDL to finish a workflow using GNN. In supervised setting, node classification aims to predict the ground truth label for each node. CogDL provides abundant of common benchmark datasets and GNN models. On the one hand, you can simply start a running using models and datasets in CogDL. This is convenient when you want to test the reproducibility of proposed GNN or get baseline results in different datasets.

```
from cogdl import experiment
experiment(model="gcn", dataset="cora")
```

Or you can create each component separately and manually run the process using `build_dataset`, `build_model` in CogDL.

```
from cogdl import experiment
from cogdl.datasets import build_dataset
from cogdl.models import build_model
from cogdl.options import get_default_args

args = get_default_args(model="gcn", dataset="cora")
dataset = build_dataset(args)
model = build_model(args)
experiment(model=model, dataset=dataset)
```

As show above, model/dataset are key components in establishing a training process. In fact, CogDL also supports customized model and datasets. This will be introduced in next chapter. In the following we will briefly show the details of each component.

2.4.4 How to save trained model?

CogDL supports saving the trained model with `checkpoint_path` in command line or API usage. For example:

```
experiment(model="gcn", dataset="cora", checkpoint_path="gcn_cora.pt")
```

When the training stops, the model will be saved in *gcn_cora.pt*. If you want to continue the training from previous checkpoint with different parameters(such as learning rate, weight decay and etc.), keep the same model parameters (such as hidden size, model layers) and do it as follows:

```
experiment(model="gcn", dataset="cora", checkpoint_path="gcn_cora.pt", resume_
↪training=True)
```

In command line usage, the same results can be achieved with `--checkpoint-path {path}` and `--resume-training`.

2.4.5 How to save embeddings?

Graph representation learning (network embedding and unsupervised GNNs) aims to get node representation. The embeddings can be used in various downstream applications. CogDL will save node embeddings in the given path specified by `--save-emb-path {path}`.

```
experiment(model="prone", dataset="blogcatalog", save_emb_path="./embeddings/prone_blog.
↪npy")
```

Evaluation on node classification will run as the end of training. We follow the same experimental settings used in DeepWalk, Node2Vec and ProNE. We randomly sample different percentages of labeled nodes for training a liblinear classifier and use the remaining for testing We repeat the training for several times and report the average Micro-F1. By default, CogDL samples 90% labeled nodes for training for one time. You are expected to change the setting with `--num-shuffle` and `--training-percents` to your needs.

In addition, CogDL supports evaluating node embeddings without training in different evaluation settings. The following code snippet evaluates the embedding we get above:

```
experiment(
    model="prone",
    dataset="blogcatalog",
    load_emb_path="./embeddings/prone_blog.npy",
    num_shuffle=5,
    training_percents=[0.1, 0.5, 0.9]
)
```

You can also use command line to achieve the same results

```
# Get embedding
python script/train.py --model prone --dataset blogcatalog

# Evaluate only
python script/train.py --model prone --dataset blogcatalog --load-emb-path ./embeddings/
↪prone_blog.npy --num-shuffle 5 --training-percents 0.1 0.5 0.9
```

2.5 Using Customized Dataset

CogDL has provided lots of common datasets. But you may wish to apply GNN to new datasets for different applications. CogDL provides an interface for customized datasets. You take care of reading in the dataset and the rest is to CogDL

We provide `NodeDataset` and `GraphDataset` as abstract classes and implement necessary basic operations.

2.5.1 Dataset for node_classification

To create a dataset for node_classification, you need to inherit `NodeDataset`. `NodeDataset` is for node-level prediction. Then you need to implement `process` method. In this method, you are expected to read in your data and preprocess raw data to the format available to CogDL with `Graph`. Afterwards, we suggest you to save the processed data (we will also help you do it as you return the data) to avoid doing the preprocessing again. Next time you run the code, CogDL will directly load it.

The running process of the module is as follows:

1. Specify the path to save processed data with *self.path*

2. Function *process* is called to load and preprocess data and your data is saved as *Graph* in *self.path*. This step will be implemented the first time you use your dataset. And then every time you use your dataset, the dataset will be loaded from *self.path* for convenience. 3. For dataset, for example, named *MyNodeDataset* in node-level tasks, You can access the data/Graph via *MyNodeDataset.data* or *MyDataset[0]*.

In addition, evaluation metric for your dataset should be specified. CogDL provides `accuracy` and `multiclass_f1` for multi-class classification, `multilabel_f1` for multi-label classification.

If `scale_feat` is set to be *True*, CogDL will normalize node features with mean *u* and variance *s*:

$$z = (x - u)/s$$

Here is an example:

```
from cogdl.data import Graph
from cogdl.datasets import NodeDataset, generate_random_graph

class MyNodeDataset(NodeDataset):
    def __init__(self, path="data.pt"):
        self.path = path
        super(MyNodeDataset, self).__init__(path, scale_feat=False, metric="accuracy")

    def process(self):
        """You need to load your dataset and transform to `Graph`"""
        num_nodes, num_edges, feat_dim = 100, 300, 30

        # load or generate your dataset
        edge_index = torch.randint(0, num_nodes, (2, num_edges))
        x = torch.randn(num_nodes, feat_dim)
        y = torch.randint(0, 2, (num_nodes,))

        # set train/val/test mask in node_classification task
        train_mask = torch.zeros(num_nodes).bool()
        train_mask[0 : int(0.3 * num_nodes)] = True
        val_mask = torch.zeros(num_nodes).bool()
        val_mask[int(0.3 * num_nodes) : int(0.7 * num_nodes)] = True
        test_mask = torch.zeros(num_nodes).bool()
        test_mask[int(0.7 * num_nodes) :] = True
        data = Graph(x=x, edge_index=edge_index, y=y, train_mask=train_mask, val_
↪mask=val_mask, test_mask=test_mask)
        return data

if __name__ == "__main__":
    # Train customized dataset via defining a new class
```

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```
    dataset = MyNodeDataset()
    experiment(dataset=dataset, model="gcn")

    # Train customized dataset via feeding the graph data to NodeDataset
    data = generate_random_graph(num_nodes=100, num_edges=300, num_feats=30)
    dataset = NodeDataset(data=data)
    experiment(dataset=dataset, model="gcn")
```

2.5.2 Dataset for graph_classification

Similarly, you need to inherit `GraphDataset` when you want to build a dataset for graph-level tasks such as *graph_classification*. The overall implementation is similar while the difference is in `process`. As `GraphDataset` contains a lot of graphs, you need to transform your data to `Graph` for each graph separately to form a list of `Graph`. An example is shown as follows:

```
from cogdl.data import Graph
from cogdl.datasets import GraphDataset

class MyGraphDataset(GraphDataset):
    def __init__(self, path="data.pt"):
        self.path = path
        super(MyGraphDataset, self).__init__(path, metric="accuracy")

    def process(self):
        # Load and preprocess data
        # Here we randomly generate several graphs for simplicity as an example
        graphs = []
        for i in range(10):
            edges = torch.randint(0, 20, (2, 30))
            label = torch.randint(0, 7, (1,))
            graphs.append(Graph(edge_index=edges, y=label))
        return graphs

if __name__ == "__main__":
    dataset = MyGraphDataset()
    experiment(model="gin", dataset=dataset)
```

2.6 Using Customized GNN

Sometimes you would like to design your own GNN module or use GNN for other purposes. In this chapter, we introduce how to use GNN layer in CogDL to write your own GNN model and how to write a GNN layer from scratch.

2.6.1 GNN layers in CogDL to Define model

CogDL has implemented popular GNN layers in `cogdl.layers`, and they can serve as modules to help design new GNNs. Here is how we implement Jumping Knowledge Network (JKNet) with `GCNLayer` in CogDL.

JKNet collects the output of all layers and concatenate them together to get the result:

$$H^{(0)} = X$$
$$H^{(i+1)} = \sigma(\hat{A}H^{(i)}W^{(i)})$$
$$OUT = CONCAT([H^{(0)}, ..., H^{(L)}])$$

```
import torch
from cogdl.layers import GCNLayer
from cogdl.models import BaseModel

class JKNet(BaseModel):
    def __init__(self, in_feats, out_feats, hidden_size, num_layers):
        super(JKNet, self).__init__()
        shapes = [in_feats] + [hidden_size] * num_layers
        self.layers = nn.ModuleList([
            GCNLayer(shape[i], shape[i+1])
            for i in range(num_layers)
        ])
        self.fc = nn.Linear(hidden_size * num_layers, out_feats)

    def forward(self, graph):
        # symmetric normalization of adjacency matrix
        graph.sym_norm()
        h = graph.x
        out = []
        for layer in self.layers:
            h = layer(x)
            out.append(h)
        out = torch.cat(out, dim=1)
        return self.fc(out)
```

2.6.2 Define your GNN Module

In most cases, you may build a layer module with new message propagation and aggragation scheme. Here the code snippet shows how to implement a GCNLayer using `Graph` and efficient sparse matrix operators in CogDL.

```
import torch
from cogdl.utils import spmm

class GCNLayer(torch.nn.Module):
```

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```
    """
    Args:
        in_feats: int
            Input feature size
        out_feats: int
            Output feature size
    """
    def __init__(self, in_feats, out_feats):
        super(GCNLayer, self).__init__()
        self.fc = torch.nn.Linear(in_feats, out_feats)

    def forward(self, graph, x):
        h = self.fc(x)
        h = spmm(graph, h)
        return h
```

`spmm` is sparse matrix multiplication operation frequently used in GNNs.

$$H = AH = spmm(A, H)$$

Sparse matrix is stored in `Graph` and will be called automatically. Message-passing in spatial space is equivalent to matrix operations. CogDL also supports other efficient operators like `edge_softmax` and `multi_head_spmm`, you can refer to this page for usage.

2.6.3 Use Custom models with CogDL

Now that you have defined your own GNN, you can use dataset/task in CogDL to immediately train and evaluate the performance of your model.

```
data = dataset.data
# Use the JKNet model as defined above
model = JKNet(data.num_features, data.num_classes, 32, 4)
experiment(model=model, dataset="cora", mw="node_classification_mw", dw="node_
↪classification_dw")
```

2.7 Experimental Results

CogDL provides 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.

2.7.1 Network embedding

Unsupervised node classification task aims to learn a mapping function that projects each node to a d-dimensional space in an unsupervised manner. Structural properties of the network should be captured by the mapping function. 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. The following table shows the results.

Rank	Method	PPI	Wikipedia	Blog-catalog	DBLP	Flickr
1	NetMF (Qiu et al, WSDM'18)	23.73 ± 0.22	57.42 ± 0.56	42.47 ± 0.35	56.72 ± 0.14	36.27 ± 0.17
2	ProNE (Zhang et al, IJCAI'19)	24.60 ± 0.39	56.06 ± 0.48	41.14 ± 0.26	56.85 ± 0.28	36.56 ± 0.11
3	NetSMF (Qiu et at, WWW'19)	23.88 ± 0.35	53.81 ± 0.58	40.62 ± 0.35	59.76 ± 0.41	35.49 ± 0.07
4	Node2vec (Grover et al, KDD'16)	20.67 ± 0.54	54.59 ± 0.51	40.16 ± 0.29	57.36 ± 0.39	36.13 ± 0.13
5	LINE (Tang et al, WWW'15)	21.82 ± 0.56	52.46 ± 0.26	38.06 ± 0.39	49.78 ± 0.37	31.61 ± 0.09
6	DeepWalk (Perozzi et al, KDD'14)	20.74 ± 0.40	49.53 ± 0.54	40.48 ± 0.47	57.54 ± 0.32	36.09 ± 0.10
7	Spectral (Tang et al, Data Min Knowl Disc (2011))	22.48 ± 0.30	49.35 ± 0.34	41.41 ± 0.34	43.68 ± 0.58	33.09 ± 0.07
8	Hope (Ou et al, KDD'16)	21.43 ± 0.32	54.04 ± 0.47	33.99 ± 0.35	56.15 ± 0.22	28.97 ± 0.19
9	GraRep (Cao et al, CIKM'15)	20.60 ± 0.34	54.37 ± 0.40	33.48 ± 0.30	52.76 ± 0.42	31.83 ± 0.12

2.7.2 Graph neural networks

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.

Rank	Method	Cora	Citeseer	Pubmed
1	Grand(Feng et al., NIPS'20)	84.8 ± 0.3	75.1 ± 0.3	82.4 ± 0.4
2	GCNII(Chen et al., ICML'20)	85.1 ± 0.3	71.3 ± 0.4	80.2 ± 0.3
3	DR-GAT (Zou et al., 2019)	83.6 ± 0.5	72.8 ± 0.8	79.1 ± 0.3
4	MVGRL (Hassani et al., KDD'20)	83.6 ± 0.2	73.0 ± 0.3	80.1 ± 0.7
5	APPNP (Klicpera et al., ICLR'19)	84.3 ± 0.8	72.0 ± 0.2	80.0 ± 0.2
6	Graph U-Net (Gao et al., 2019)	83.3 ± 0.3	71.2 ± 0.4	79.0 ± 0.7
7	GAT (Veličković et al., ICLR'18)	82.9 ± 0.8	71.0 ± 0.3	78.9 ± 0.3
8	GDC_GCN (Klicpera et al., NeurIPS'19)	82.5 ± 0.4	71.2 ± 0.3	79.8 ± 0.5
9	DropEdge(Rong et al., ICLR'20)	82.1 ± 0.5	72.1 ± 0.4	79.7 ± 0.4
10	GCN (Kipf et al., ICLR'17)	82.3 ± 0.3	71.4 ± 0.4	79.5 ± 0.2
11	DGI (Veličković et al., ICLR'19)	82.0 ± 0.2	71.2 ± 0.4	76.5 ± 0.6
12	JK-net (Xu et al., ICML'18)	81.8 ± 0.2	69.5 ± 0.4	77.7 ± 0.6
13	GraphSAGE (Hamilton et al., NeurIPS'17)	80.1 ± 0.2	66.2 ± 0.4	77.2 ± 0.7
14	GraphSAGE(unsup)(Hamilton et al., NeurIPS'17)	78.2 ± 0.9	65.8 ± 1.0	78.2 ± 0.7
15	Chebyshev (Defferrard et al., NeurIPS'16)	79.0 ± 1.0	69.8 ± 0.5	68.6 ± 1.0
16	MixHop (Abu-El-Haija et al., ICML'19)	81.9 ± 0.4	71.4 ± 0.8	80.8 ± 0.6

2.8 data

class cogdl.data.**Adjacency**(*row=None*, *col=None*, *row_ptr=None*, *weight=None*, *attr=None*, *num_nodes=None*, *types=None*, ***kwargs*)

Bases: `cogdl.data.data.BaseGraph`

add_remaining_self_loops()

clone()

col_norm()

convert_csr()

degrees(*node_idx=None*)

property device

property edge_index

static from_dict(*dictionary*)
Creates a data object from a python dictionary.

generate_normalization(*norm='sym'*)

get_weight(*indicator=None*)
If *indicator* is not None, the normalization will not be implemented

is_symmetric()

property keys
Returns all names of graph attributes.

normalize_adj(*norm='sym'*)

property **num_edges**

property **num_nodes**

padding_self_loops()

random_walk(*seeds*, *length=1*, *restart_p=0.0*)

remove_self_loops()

property **row_indptr**

row_norm()

property **row_ptr_v**

set_symmetric(*val*)

set_weight(*weight*)

sym_norm()

to_networkx(*weighted=True*)

to_scipy_csr()

class cogdl.data.**Batch**(*batch=None*, ***kwargs*)

Bases: *cogdl.data.data.Graph*

A plain old python object modeling a batch of graphs as one big (dicconnected) graph. With `cogdl.data.Data` being the base class, all its methods can also be used here. In addition, single graphs can be reconstructed via the assignment vector `batch`, which maps each node to its respective graph identifier.

cumsum(*key*, *item*)

If `True`, the attribute `key` with content `item` should be added up cumulatively before concatenated together.

Note: This method is for internal use only, and should only be overridden if the batch concatenation process is corrupted for a specific data attribute.

static **from_data_list**(*data_list*, *class_type=None*)

Constructs a batch object from a python list holding `cogdl.data.Data` objects. The assignment vector `batch` is created on the fly. Additionally, creates assignment batch vectors for each key in `follow_batch`.

property **num_graphs**

Returns the number of graphs in the batch.

class cogdl.data.**DataLoader**(**args*, ***kwargs*)

Bases: `Generic`[`torch.utils.data.dataloader.T_co`]

Data loader which merges data objects from a `cogdl.data.dataset` to a mini-batch.

Parameters

- **dataset** (`Dataset`) – The dataset from which to load the data.
- **batch_size** (*int, optional*) – How may samples per batch to load. (default: `1`)
- **shuffle** (*bool, optional*) – If set to `True`, the data will be reshuffled at every epoch (default: `True`)

batch_size: Optional[int]

static **collate_fn**(*batch*)

dataset: torch.utils.data.dataset.Dataset[torch.utils.data.dataloader.T_co]

drop_last: bool

get_parameters()

num_workers: int

pin_memory: bool

prefetch_factor: int

record_parameters(*params*)

sampler: torch.utils.data.sampler.Sampler

timeout: float

class cogdl.data.**Dataset**(*root*, *transform=None*, *pre_transform=None*, *pre_filter=None*)

Bases: Generic[torch.utils.data.dataset.T_co]

Dataset base class for creating graph datasets.

Parameters

- **root** (*string*) – Root directory where the dataset should be saved.
- **transform** (*callable, optional*) – A function/transform that takes in an cogdl.data.Data object and returns a transformed version. The data object will be transformed before every access. (default: None)
- **pre_transform** (*callable, optional*) – A function/transform that takes in an cogdl.data.Data object and returns a transformed version. The data object will be transformed before being saved to disk. (default: None)
- **pre_filter** (*callable, optional*) – A function that takes in an cogdl.data.Data object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: None)

static add_args(*parser*)

Add dataset-specific arguments to the parser.

download()

Downloads the dataset to the self.raw_dir folder.

property edge_attr_size

get(*idx*)

Gets the data object at index idx.

get_evaluator()

get_loss_fn()

property max_degree

property max_graph_size

property num_classes

The number of classes in the dataset.

property num_features

Returns the number of features per node in the graph.

property num_graphs

process()
Processes the dataset to the `self.processed_dir` folder.

property processed_file_names
The name of the files to find in the `self.processed_dir` folder in order to skip the processing.

property processed_paths
The filepaths to find in the `self.processed_dir` folder in order to skip the processing.

property raw_file_names
The name of the files to find in the `self.raw_dir` folder in order to skip the download.

property raw_paths
The filepaths to find in order to skip the download.

class cogdl.data.**Graph**(*x=None*, *y=None*, ***kwargs*)
Bases: `cogdl.data.data.BaseGraph`

add_remaining_self_loops()

clone()

property col_indices

col_norm()

csr_subgraph(*node_idx*, *keep_order=False*)

degrees()

property device

property edge_attr

property edge_index

edge_subgraph(*edge_idx*, *require_idx=True*)

property edge_types

property edge_weight
Return actual edge_weight

eval()

static from_dict(*dictionary*)
Creates a data object from a python dictionary.

static from_pyg_data(*data*)

property in_norm

is_inductive()

is_symmetric()

property keys
Returns all names of graph attributes.

local_graph()

mask2nid(*split*)

nodes()

normalize(*key='sym'*)

property num_classes

property num_edges
Returns the number of edges in the graph.

property num_features
Returns the number of features per node in the graph.

property num_nodes

property out_norm

padding_self_loops()

random_walk(*seeds*, *max_nodes_per_seed*, *restart_p=0.0*)

random_walk_with_restart(*seeds*, *max_nodes_per_seed*, *restart_p=0.0*)

property raw_edge_weight
Return edge_weight without __in_norm__ and __out_norm__, only used for SpMM

remove_self_loops()

restore(*key*)

property row_indptr

row_norm()

sample_adj(*batch*, *size=- 1*, *replace=True*)

set_asymmetric()

set_symmetric()

store(*key*)

subgraph(*node_idx*, *keep_order=False*)

sym_norm()

property test_nid

to_networkx()

to_scipy_csr()

train()

property train_nid

property val_nid

class cogdl.data.**MultiGraphDataset**(*root=None*, *transform=None*, *pre_transform=None*, *pre_filter=None*)
Bases: Generic[torch.utils.data.dataset.T_co]

get(*idx*)
Gets the data object at index `idx`.

len()

property max_degree

property max_graph_size

property num_classes
The number of classes in the dataset.

property num_features
Returns the number of features per node in the graph.

property num_graphs

cogdl.data.**batch_graphs**(*graphs*)

2.9 datasets

2.9.1 GATNE dataset

class cogdl.datasets.gatne.**AmazonDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.gatne.**GatneDataset**(*root*, *name*)
Bases: Generic[torch.utils.data.dataset.T_co]

The network datasets "Amazon", "Twitter" and "YouTube" from the "Representation Learning for Attributed Multiplex Heterogeneous Network" paper.

Parameters

- **root** (*string*) – Root directory where the dataset should be saved.
- **name** (*string*) – The name of the dataset ("Amazon", "Twitter", "YouTube").

download()
Downloads the dataset to the self.raw_dir folder.

get(*idx*)
Gets the data object at index idx.

process()
Processes the dataset to the self.processed_dir folder.

property processed_file_names
The name of the files to find in the self.processed_dir folder in order to skip the processing.

property raw_file_names
The name of the files to find in the self.raw_dir folder in order to skip the download.

url = 'https://github.com/THUDM/GATNE/raw/master/data'

class cogdl.datasets.gatne.**TwitterDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.gatne.**YouTubeDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

cogdl.datasets.gatne.**read_gatne_data**(*folder*)

2.9.2 GCC dataset

class cogdl.datasets.gcc_data.**Edgelist**(*root*, *name*)
Bases: Generic[torch.utils.data.dataset.T_co]

download()
Downloads the dataset to the self.raw_dir folder.

get(*idx*)
Gets the data object at index idx.

property num_classes
The number of classes in the dataset.

process()
Processes the dataset to the `self.processed_dir` folder.

property processed_file_names
The name of the files to find in the `self.processed_dir` folder in order to skip the processing.

property raw_file_names
The name of the files to find in the `self.raw_dir` folder in order to skip the download.

url = 'https://github.com/cenyk1230/gcc-data/raw/master'

class cogdl.datasets.gcc_data.**GCCDataset**(*root*, *name*)
Bases: Generic[torch.utils.data.dataset.T_co]

download()
Downloads the dataset to the `self.raw_dir` folder.

get(*idx*)
Gets the data object at index `idx`.

preprocess(*root*, *name*)

property processed_file_names
The name of the files to find in the `self.processed_dir` folder in order to skip the processing.

property raw_file_names
The name of the files to find in the `self.raw_dir` folder in order to skip the download.

url = 'https://github.com/cenyk1230/gcc-data/raw/master'

class cogdl.datasets.gcc_data.**KDD_ICDM_GCCDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.gcc_data.**SIGIR_CIKM_GCCDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.gcc_data.**SIGMOD_ICDE_GCCDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.gcc_data.**USAAirportDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

2.9.3 GTN dataset

class cogdl.datasets.gtn_data.**ACM_GTNDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.gtn_data.**DBLP_GTNDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.gtn_data.**GTNDataset**(*root*, *name*)
Bases: Generic[torch.utils.data.dataset.T_co]

The network datasets "ACM", "DBLP" and "IMDB" from the "Graph Transformer Networks" paper.

Parameters

- **root** (*string*) – Root directory where the dataset should be saved.
- **name** (*string*) – The name of the dataset ("gtn-acm", "gtn-dblp", "gtn-imdb").

apply_to_device(*device*)

download()
Downloads the dataset to the `self.raw_dir` folder.

get(*idx*)
Gets the data object at index `idx`.

property num_classes
The number of classes in the dataset.

process()
Processes the dataset to the `self.processed_dir` folder.

property processed_file_names
The name of the files to find in the `self.processed_dir` folder in order to skip the processing.

property raw_file_names
The name of the files to find in the `self.raw_dir` folder in order to skip the download.

read_gtn_data(*folder*)

class cogdl.datasets.gtn_data.**IMDB_GTNDataset**(*data_path='data'*)
Bases: Generic[`torch.utils.data.dataset.T_co`]

2.9.4 HAN dataset

class cogdl.datasets.han_data.**ACM_HANDataset**(*data_path='data'*)
Bases: Generic[`torch.utils.data.dataset.T_co`]

class cogdl.datasets.han_data.**DBLP_HANDataset**(*data_path='data'*)
Bases: Generic[`torch.utils.data.dataset.T_co`]

class cogdl.datasets.han_data.**HANDataset**(*root*, *name*)
Bases: Generic[`torch.utils.data.dataset.T_co`]

The network datasets "ACM", "DBLP" and "IMDB" from the "Heterogeneous Graph Attention Network" paper.

Parameters

- **root** (*string*) – Root directory where the dataset should be saved.
- **name** (*string*) – The name of the dataset (`"han-acm"`, `"han-dblp"`, `"han-imdb"`).

apply_to_device(*device*)

download()
Downloads the dataset to the `self.raw_dir` folder.

get(*idx*)
Gets the data object at index `idx`.

property num_classes
The number of classes in the dataset.

process()
Processes the dataset to the `self.processed_dir` folder.

property processed_file_names
The name of the files to find in the `self.processed_dir` folder in order to skip the processing.

property raw_file_names
The name of the files to find in the `self.raw_dir` folder in order to skip the download.

read_gtn_data(*folder*)

class cogdl.datasets.han_data.**IMDB_HANDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

cogdl.datasets.han_data.**sample_mask**(*idx*, *length*)
Create mask.

2.9.5 KG dataset

class cogdl.datasets.kg_data.**FB13Datset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.kg_data.**FB13SDatset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.kg_data.**FB15k237Datset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.kg_data.**FB15kDatset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.kg_data.**KnowledgeGraphDataset**(*root*, *name*)
Bases: Generic[torch.utils.data.dataset.T_co]

download()
Downloads the dataset to the `self.raw_dir` folder.

get(*idx*)
Gets the data object at index `idx`.

property num_entities

property num_relations

process()
Processes the dataset to the `self.processed_dir` folder.

property processed_file_names
The name of the files to find in the `self.processed_dir` folder in order to skip the processing.

property raw_file_names
The name of the files to find in the `self.raw_dir` folder in order to skip the download.

property test_start_idx

property train_start_idx

url = 'https://cloud.tsinghua.edu.cn/d/d1c733373b014efab986/files/?p=%2F{}%2F{}&dl=1'

property valid_start_idx

class cogdl.datasets.kg_data.**WN18Datset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.kg_data.**WN18RRDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

cogdl.datasets.kg_data.**read_triplet_data**(*folder*)

2.9.6 Matlab matrix dataset

class cogdl.datasets.matlab_matrix.**BlogcatalogDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.matlab_matrix.**DblpNEDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.matlab_matrix.**FlickrDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.matlab_matrix.**MatlabMatrix**(*root*, *name*, *url*)
Bases: Generic[torch.utils.data.dataset.T_co]

networks from the http://leitang.net/code/social-dimension/data/ or http://snap.stanford.edu/node2vec/

Parameters

- **root** (*string*) – Root directory where the dataset should be saved.
- **name** (*string*) – The name of the dataset ("Blogcatalog").

download()
Downloads the dataset to the self.raw_dir folder.

get(*idx*)
Gets the data object at index idx.

property **num_classes**
The number of classes in the dataset.

property **num_nodes**

process()
Processes the dataset to the self.processed_dir folder.

property **processed_file_names**
The name of the files to find in the self.processed_dir folder in order to skip the processing.

property **raw_file_names**
The name of the files to find in the self.raw_dir folder in order to skip the download.

class cogdl.datasets.matlab_matrix.**NetworkEmbeddingCMTYDataset**(*root*, *name*, *url*)
Bases: Generic[torch.utils.data.dataset.T_co]

download()
Downloads the dataset to the self.raw_dir folder.

get(*idx*)
Gets the data object at index idx.

property **num_classes**
The number of classes in the dataset.

property **num_nodes**

process()
Processes the dataset to the self.processed_dir folder.

property **processed_file_names**
The name of the files to find in the self.processed_dir folder in order to skip the processing.

property **raw_file_names**
The name of the files to find in the self.raw_dir folder in order to skip the download.

class cogdl.datasets.matlab_matrix.**PPIDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.matlab_matrix.**WikipediaDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.matlab_matrix.**YoutubeNEDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

2.9.7 OGB dataset

class cogdl.datasets.ogb.**OGBArxivDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBCodeDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBGDataset**(*root*, *name*)
Bases: Generic[torch.utils.data.dataset.T_co]

get(*idx*)
Gets the data object at index idx.

get_loader(*args*)

get_subset(*subset*)

property num_classes
The number of classes in the dataset.

class cogdl.datasets.ogb.**OGBMolbaceDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBMolhivDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBMolpcbaDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBNDataset**(*root*, *name*, *transform=None*)
Bases: Generic[torch.utils.data.dataset.T_co]

get(*idx*)
Gets the data object at index idx.

get_evaluator()

get_loss_fn()

process()
Processes the dataset to the self.processed_dir folder.

property processed_file_names
The name of the files to find in the self.processed_dir folder in order to skip the processing.

class cogdl.datasets.ogb.**OGBPapers100MDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBPpaDataset**
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBProductsDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.ogb.**OGBProteinsDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

property edge_attr_size

get_evaluator()

get_loss_fn()

process()
Processes the dataset to the `self.processed_dir` folder.

2.9.8 TU dataset

class cogdl.datasets.tu_data.**CollabDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**ENZYMES**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**ImdbBinaryDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**ImdbMultiDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**MUTAGDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**NCI109Dataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**NCI1Dataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**PTCMRDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**ProteinsDataset**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**RedditBinary**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**RedditMulti12K**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**RedditMulti5K**(*data_path='data'*)
Bases: Generic[torch.utils.data.dataset.T_co]

class cogdl.datasets.tu_data.**TUDataset**(*root*, *name*)
Bases: Generic[torch.utils.data.dataset.T_co]

download()
Downloads the dataset to the `self.raw_dir` folder.

property num_classes
The number of classes in the dataset.

process()
Processes the dataset to the `self.processed_dir` folder.

property processed_file_names
The name of the files to find in the `self.processed_dir` folder in order to skip the processing.

property raw_file_names
The name of the files to find in the `self.raw_dir` folder in order to skip the download.

url = 'https://www.chrsmrrs.com/graphkerneldatasets'

cogdl.datasets.tu_data.**cat**(*seq*)

cogdl.datasets.tu_data.**coalesce**(*index*, *value*, *m*, *n*)

cogdl.datasets.tu_data.**normalize_feature**(*data*)

cogdl.datasets.tu_data.**num_edge_attributes**(*edge_attr=None*)

cogdl.datasets.tu_data.**num_edge_labels**(*edge_attr=None*)

cogdl.datasets.tu_data.**num_node_attributes**(*x=None*)

cogdl.datasets.tu_data.**num_node_labels**(*x=None*)

cogdl.datasets.tu_data.**parse_txt_array**(*src*, *sep=None*, *start=0*, *end=None*, *dtype=None*, *device=None*)

cogdl.datasets.tu_data.**read_file**(*folder*, *prefix*, *name*, *dtype=None*)

cogdl.datasets.tu_data.**read_tu_data**(*folder*, *prefix*)

cogdl.datasets.tu_data.**read_txt_array**(*path*, *sep=None*, *start=0*, *end=None*, *dtype=None*, *device=None*)

cogdl.datasets.tu_data.**segment**(*src*, *indptr*)

2.9.9 Module contents

cogdl.datasets.**build_dataset**(*args*)

cogdl.datasets.**build_dataset_from_name**(*dataset*, *split=0*)

cogdl.datasets.**build_dataset_from_path**(*data_path*, *dataset=None*)

cogdl.datasets.**register_dataset**(*name*)
New dataset types can be added to cogdl with the `register_dataset()` function decorator.

For example:

```
@register_dataset('my_dataset')
class MyDataset():
    (...)
```

Parameters **name** (*str*) – the name of the dataset

cogdl.datasets.**try_adding_dataset_args**(*dataset*, *parser*)

2.10 models

2.10.1 BaseModel

class cogdl.models.base_model.**BaseModel**
Bases: torch.nn.modules.module.Module

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)
Build a new model instance.

property device

forward(**args*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

predict(*data*)

set_loss_fn(*loss_fn*)

training: bool

2.10.2 Embedding Model

class cogdl.models.emb.hope.**HOPE**(*dimension*, *beta*)
Bases: *cogdl.models.base_model.BaseModel*

The HOPE model from the "Grarep: Asymmetric transitivity preserving graph embedding" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **beta** (*float*) – Parameter in katz decomposition.

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*, *return_dict=False*)
The author claim that Katz has superior performance in related tasks S_katz = (M_g)^-1 * M_l = (I - beta*A)^-1 * beta*A = (I - beta*A)^-1 * (I - (I -beta*A)) = (I - beta*A)^-1 - I

training: bool

class cogdl.models.emb.spectral.**Spectral**(*hidden_size*)
Bases: *cogdl.models.base_model.BaseModel*

The Spectral clustering model from the "Leveraging social media networks for classication" paper

Parameters hidden_size (*int*) – The dimension of node representation.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*, *return_dict=False*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.models.emb.hin2vec.**Hin2vec**(*hidden_dim*, *walk_length*, *walk_num*, *batch_size*, *hop*, *negative*, *epochs*, *lr*, *cpu=True*)

Bases: *cogdl.models.base_model.BaseModel*

The Hin2vec model from the "HIN2Vec: Explore Meta-paths in Heterogeneous Information Networks for Representation Learning" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **walk_length** (*int*) – The walk length.
- **walk_num** (*int*) – The number of walks to sample for each node.
- **batch_size** (*int*) – The batch size of training in Hin2vec.
- **hop** (*int*) – The number of hop to construct training samples in Hin2vec.
- **negative** (*int*) – The number of nagative samples for each meta2path pair.
- **epochs** (*int*) – The number of training iteration.
- **lr** (*float*) – The initial learning rate of SGD.
- **cpu** (*bool*) – Use CPU or GPU to train hin2vec.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*data*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.models.emb.netmf.**NetMF**(*dimension*, *window_size*, *rank*, *negative*, *is_large=False*)

Bases: *cogdl.models.base_model.BaseModel*

The NetMF model from the "Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **window_size** (*int*) – The actual context size which is considered in language model.
- **rank** (*int*) – The rank in approximate normalized laplacian.
- **negative** (*int*) – The number of nagative samples in negative sampling.
- **is-large** (*bool*) – When window size is large, use approximated deepwalk matrix to decompose.

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*, *return_dict=False*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.deepwalk.DeepWalk(*dimension*, *walk_length*, *walk_num*, *window_size*, *worker*, *iteration*)
Bases: *cogdl.models.base_model.BaseModel*

The DeepWalk model from the "DeepWalk: Online Learning of Social Representations" paper

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **walk_length** (*int*) – The walk length.
- **walk_num** (*int*) – The number of walks to sample for each node.
- **window_size** (*int*) – The actual context size which is considered in language model.
- **worker** (*int*) – The number of workers for word2vec.
- **iteration** (*int*) – The number of training iteration in word2vec.

static add_args(*parser: argparse.ArgumentParser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*) → *cogdl.models.emb.deepwalk.DeepWalk*

forward(*graph*, *embedding_model_creator=<class 'gensim.models.word2vec.Word2Vec'>*, *return_dict=False*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.gatne.**GATNE**(*dimension*, *walk_length*, *walk_num*, *window_size*, *worker*, *epochs*, *batch_size*, *edge_dim*, *att_dim*, *negative_samples*, *neighbor_samples*, *schema*)

Bases: *cogdl.models.base_model.BaseModel*

The GATNE model from the "Representation Learning for Attributed Multiplex Heterogeneous Network" paper

Parameters

- **walk_length** (*int*) – The walk length.
- **walk_num** (*int*) – The number of walks to sample for each node.
- **window_size** (*int*) – The actual context size which is considered in language model.
- **worker** (*int*) – The number of workers for word2vec.
- **epochs** (*int*) – The number of training epochs.
- **batch_size** (*int*) – The size of each training batch.
- **edge_dim** (*int*) – Number of edge embedding dimensions.
- **att_dim** (*int*) – Number of attention dimensions.
- **negative_samples** (*int*) – Negative samples for optimization.
- **neighbor_samples** (*int*) – Neighbor samples for aggregation
- **schema** (*str*) – The metapath schema used in model. Metapaths are splited with ",",
- **example** (*while each node type are connected with "-" in each metapath. For*) – "0-1-0,0-1-2-1-0"

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*network_data*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.dgk.**DeepGraphKernel**(*hidden_dim*, *min_count*, *window_size*, *sampling_rate*, *rounds*, *epochs*, *alpha*, *n_workers=4*)

Bases: *cogdl.models.base_model.BaseModel*

The Hin2vec model from the "Deep Graph Kernels" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **min_count** (*int*) – Parameter in word2vec.
- **window** (*int*) – The actual context size which is considered in language model.
- **sampling_rate** (*float*) – Parameter in word2vec.
- **iteration** (*int*) – The number of iteration in WL method.
- **epochs** (*int*) – The number of training iteration.
- **alpha** (*float*) – The learning rate of word2vec.

static **add_args**(*parser*)
Add model-specific arguments to the parser.

classmethod **build_model_from_args**(*args*)

static **feature_extractor**(*data*, *rounds*, *name*)

forward(*graphs*, ***kwargs*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

save_embedding(*output_path*)

training: bool

static **wl_iterations**(*graph*, *features*, *rounds*)

class cogdl.models.emb.grarep.**GraRep**(*dimension*, *step*)
Bases: *cogdl.models.base_model.BaseModel*

The GraRep model from the "Grarep: Learning graph representations with global structural information" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **step** (*int*) – The maximum order of transitition probability.

static **add_args**(*parser*)
Add model-specific arguments to the parser.

classmethod **build_model_from_args**(*args*)

forward(*graph*, *return_dict=False*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.dngr.**DNGR**(*hidden_size1*, *hidden_size2*, *noise*, *alpha*, *step*, *epochs*, *lr*, *cpu*)

Bases: *cogdl.models.base_model.BaseModel*

The DNGR model from the "Deep Neural Networks for Learning Graph Representations" paper

Parameters

- **hidden_size1** (*int*) – The size of the first hidden layer.
- **hidden_size2** (*int*) – The size of the second hidden layer.
- **noise** (*float*) – Denoise rate of DAE.
- **alpha** (*float*) – Parameter in DNGR.
- **step** (*int*) – The max step in random surfing.
- **epochs** (*int*) – The max epoches in training step.
- **lr** (*float*) – Learning rate in DNGR.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*, *return_dict=False*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

get_denoised_matrix(*mat*)

get_emb(*matrix*)

get_ppmi_matrix(*mat*)

random_surfing(*adj_matrix*)

scale_matrix(*mat*)

training: bool

class cogdl.models.emb.pronepp.**ProNEPP**(*filter_types*, *svd*, *search*, *max_evals=None*, *loss_type=None*, *n_workers=None*)

Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

training: bool

class cogdl.models.emb.graph2vec.**Graph2Vec**(*dimension*, *min_count*, *window_size*, *dm*, *sampling_rate*, *rounds*, *epochs*, *lr*, *worker=4*)

Bases: *cogdl.models.base_model.BaseModel*

The Graph2Vec model from the "graph2vec: Learning Distributed Representations of Graphs" paper

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **min_count** (*int*) – Parameter in doc2vec.
- **window_size** (*int*) – The actual context size which is considered in language model.
- **sampling_rate** (*float*) – Parameter in doc2vec.
- **dm** (*int*) – Parameter in doc2vec.
- **iteration** (*int*) – The number of iteration in WL method.
- **lr** (*float*) – Learning rate in doc2vec.

static **add_args**(*parser*)
Add model-specific arguments to the parser.

classmethod **build_model_from_args**(*args*)

static **feature_extractor**(*data*, *rounds*, *name*)

forward(*graphs*, ***kwargs*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

save_embedding(*output_path*)

training: bool

static **wl_iterations**(*graph*, *features*, *rounds*)

class cogdl.models.emb.metapath2vec.**Metapath2vec**(*dimension*, *walk_length*, *walk_num*, *window_size*, *worker*, *iteration*, *schema*)
Bases: `cogdl.models.base_model.BaseModel`

The Metapath2vec model from the "metapath2vec: Scalable Representation Learning for Heterogeneous Networks" paper

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **walk_length** (*int*) – The walk length.
- **walk_num** (*int*) – The number of walks to sample for each node.
- **window_size** (*int*) – The actual context size which is considered in language model.
- **worker** (*int*) – The number of workers for word2vec.
- **iteration** (*int*) – The number of training iteration in word2vec.
- **schema** (*str*) – The metapath schema used in model. Metapaths are splited with ",",
- **example** (*while each node type are connected with "-" in each metapath. For*) – "0-1-0,0-2-0,1-0-2-0-1".

static **add_args**(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*data*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.models.emb.node2vec.Node2vec(*dimension, walk_length, walk_num, window_size, worker, iteration, p, q*)

Bases: `cogdl.models.base_model.BaseModel`

The node2vec model from the "node2vec: Scalable feature learning for networks" paper

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **walk_length** (*int*) – The walk length.
- **walk_num** (*int*) – The number of walks to sample for each node.
- **window_size** (*int*) – The actual context size which is considered in language model.
- **worker** (*int*) – The number of workers for word2vec.
- **iteration** (*int*) – The number of training iteration in word2vec.
- **p** (*float*) – Parameter in node2vec.
- **q** (*float*) – Parameter in node2vec.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph, return_dict=False*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.models.emb.pte.PTE(*dimension, walk_length, walk_num, negative, batch_size, alpha*)

Bases: `cogdl.models.base_model.BaseModel`

The PTE model from the "PTE: Predictive Text Embedding through Large-scale Heterogeneous Text Networks" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.

- **walk_length** (*int*) – The walk length.
- **walk_num** (*int*) – The number of walks to sample for each node.
- **negative** (*int*) – The number of nagative samples for each edge.
- **batch_size** (*int*) – The batch size of training in PTE.
- **alpha** (*float*) – The initial learning rate of SGD.

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*data*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.netsmf.**NetSMF**(*dimension*, *window_size*, *negative*, *num_round*, *worker*)
Bases: *cogdl.models.base_model.BaseModel*

The NetSMF model from the "NetSMF: Large-Scale Network Embedding as Sparse Matrix Factorization" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **window_size** (*int*) – The actual context size which is considered in language model.
- **negative** (*int*) – The number of nagative samples in negative sampling.
- **num_round** (*int*) – The number of round in NetSMF.
- **worker** (*int*) – The number of workers for NetSMF.

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*, *return_dict=False*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.line.**LINE**(*dimension*, *walk_length*, *walk_num*, *negative*, *batch_size*, *alpha*, *order*)
Bases: *cogdl.models.base_model.BaseModel*

The LINE model from the "Line: Large-scale information network embedding" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **walk_length** (*int*) – The walk length.
- **walk_num** (*int*) – The number of walks to sample for each node.
- **negative** (*int*) – The number of nagative samples for each edge.
- **batch_size** (*int*) – The batch size of training in LINE.
- **alpha** (*float*) – The initial learning rate of SGD.
- **order** (*int*) – 1 represents perserving 1-st order proximity, 2 represents 2-nd,
- **them** (*while 3 means both of*) –

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*, *return_dict=False*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.sdne.SDNE(*hidden_size1*, *hidden_size2*, *droput*, *alpha*, *beta*, *nu1*, *nu2*, *epochs*, *lr*, *cpu*)

Bases: `cogdl.models.base_model.BaseModel`

The SDNE model from the "Structural Deep Network Embedding" paper

Parameters

- **hidden_size1** (*int*) – The size of the first hidden layer.
- **hidden_size2** (*int*) – The size of the second hidden layer.
- **droput** (*float*) – Droput rate.
- **alpha** (*float*) – Trade-off parameter between 1-st and 2-nd order objective function in SDNE.
- **beta** (*float*) – Parameter of 2-nd order objective function in SDNE.
- **nu1** (*float*) – Parameter of l1 normlization in SDNE.
- **nu2** (*float*) – Parameter of l2 normlization in SDNE.
- **epochs** (*int*) – The max epoches in training step.
- **lr** (*float*) – Learning rate in SDNE.
- **cpu** (*bool*) – Use CPU or GPU to train hin2vec.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*, *return_dict=False*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.emb.prone.**ProNE**(*dimension*, *step*, *mu*, *theta*)
Bases: *cogdl.models.base_model.BaseModel*

The ProNE model from the "ProNE: Fast and Scalable Network Representation Learning" paper.

Parameters

- **hidden_size** (*int*) – The dimension of node representation.
- **step** (*int*) – The number of items in the chebyshev expansion.
- **mu** (*float*) – Parameter in ProNE.
- **theta** (*float*) – Parameter in ProNE.

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph: cogdl.data.data.Graph*, *return_dict=False*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

2.10.3 GNN Model

class cogdl.models.nn.dgi.**DGIModel**(*in_feats*, *hidden_size*, *activation*)
Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

embed(*data*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.nn.mvgrl.**MVGRL**(*in_feats*, *hidden_size*, *sample_size=2000*, *batch_size=4*, *alpha=0.2*, *dataset='cora'*)

Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)
Add model-specific arguments to the parser.

augment(*graph*)

classmethod build_model_from_args(*args*)

embed(*data*, *msk=None*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

loss(*data*)

preprocess(*graph*)

training: bool

class cogdl.models.nn.patchy_san.**PatchySAN**(*num_features*, *num_classes*, *num_sample*, *num_neighbor*, *iteration*)

Bases: *cogdl.models.base_model.BaseModel*

The Patchy-SAN model from the "Learning Convolutional Neural Networks for Graphs" paper.

Parameters

- **batch_size** (*int*) – The batch size of training.
- **sample** (*int*) – Number of chosen vertexes.
- **stride** (*int*) – Node selection stride.
- **neighbor** (*int*) – The number of neighbor for each node.
- **iteration** (*int*) – The number of training iteration.

static add_args(*parser*)
Add model-specific arguments to the parser.

build_model(*num_channel*, *num_sample*, *num_neighbor*, *num_class*)

classmethod build_model_from_args(*args*)

forward(*batch*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

classmethod split_dataset(*dataset, args*)

training: bool

class cogdl.models.nn.gcn.**GCN**(*in_feats, hidden_size, out_feats, num_layers, dropout, activation='relu', residual=False, norm=None*)

Bases: `cogdl.models.base_model.BaseModel`

The GCN model from the "Semi-Supervised Classification with Graph Convolutional Networks" paper

Parameters

- **in_features** (*int*) – Number of input features.
- **out_features** (*int*) – Number of classes.
- **hidden_size** (*int*) – The dimension of node representation.
- **dropout** (*float*) – Dropout rate for model training.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

embed(*graph*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.models.nn.gdc_gcn.**GDC_GCN**(*nfeat, nhid, nclass, dropout, alpha, t, k, eps, gdctype*)

Bases: `cogdl.models.base_model.BaseModel`

The GDC model from the "Diffusion Improves Graph Learning" paper, with the PPR and heat matrix variants combined with GCN

Parameters

- **num_features** (*int*) – Number of input features in ppr-preprocessed dataset.
- **num_classes** (*int*) – Number of classes.
- **hidden_size** (*int*) – The dimension of node representation.
- **dropout** (*float*) – Dropout rate for model training.
- **alpha** (*float*) – PPR polynomial filter param, 0 to 1.
- **t** (*float*) – Heat polynomial filter param

- **k** (*int*) – Top k nodes retained during sparsification.
- **eps** (*float*) – Threshold for clipping.
- **gdc_type** (*str*) – "none", "ppr", "heat"

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*data=None*)

preprocessing(*data*, *gdc_type='ppr'*)

reset_data(*data*)

training: bool

class cogdl.models.nn.graphsage.**Graphsage**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *sample_size*, *dropout*, *aggr*)
Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(**args*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

inference(*x_all*, *data_loader*)

mini_forward(*graph*)

sampling(*edge_index*, *num_sample*)

training: bool

class cogdl.models.nn.compgcn.**LinkPredictCompGCN**(*num_entities*, *num_rels*, *hidden_size*, *num_bases=0*, *layers=1*, *sampling_rate=0.01*, *penalty=0.001*, *dropout=0.0*, *lbl_smooth=0.1*, *opn='sub'*)
Bases: *cogdl.utils.link_prediction_utils.GNNLinkPredict*, *cogdl.models.base_model.BaseModel*

static add_args(*parser*)
Add model-specific arguments to the parser.

add_reverse_edges(*edge_index*, *edge_types*)

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

loss(*data: cogdl.data.data.Graph*, *scoring*)

predict(*graph*)

training: bool

class cogdl.models.nn.drgcn.**DrGCN**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*, *norm=None*, *activation='relu'*)
Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*graph*)

training: bool

class cogdl.models.nn.graph_unet.**GraphUnet**(*in_feats: int*, *hidden_size: int*, *out_feats: int*, *pooling_layer: int*, *pooling_rates: List[float]*, *n_dropout: float = 0.5*, *adj_dropout: float = 0.3*, *activation: str = 'elu'*, *improved: bool = False*, *aug_adj: bool = False*)
Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph: cogdl.data.data.Graph*) → torch.Tensor
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.nn.gcnmix.**GCNMix**(*in_feat*, *hidden_size*, *num_classes*, *k*, *temperature*, *alpha*, *dropout*)
Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

forward_aux(*x*, *label*, *train_index*, *mix_hidden=True*, *layer_mix=1*)

predict_noise(*data*, *tau=1*)

training: bool

class cogdl.models.nn.diffpool.**DiffPool**(*in_feats*, *hidden_dim*, *embed_dim*, *num_classes*, *num_layers*, *num_pool_layers*, *assign_dim*, *pooling_ratio*, *batch_size*, *dropout=0.5*, *no_link_pred=True*, *concat=False*, *use_bn=False*)
Bases: `cogdl.models.base_model.BaseModel`

DIFFPOOL from paper Hierarchical Graph Representation Learning with Differentiable Pooling.

Parameters

- **in_feats** (*int*) – Size of each input sample.
- **hidden_dim** (*int*) – Size of hidden layer dimension of GNN.
- **embed_dim** (*int*) – Size of embeded node feature, output size of GNN.
- **num_classes** (*int*) – Number of target classes.
- **num_layers** (*int*) – Number of GNN layers.
- **num_pool_layers** (*int*) – Number of pooling.
- **assign_dim** (*int*) – Embedding size after the first pooling.
- **pooling_ratio** (*float*) – Size of each poolling ratio.
- **batch_size** (*int*) – Size of each mini-batch.
- **dropout** (*float, optional*) – Size of dropout, default: *0.5*.
- **no_link_pred** (*bool, optional*) – If True, use link prediction loss, default: *True*.

static add_args(*parser*)
Add model-specific arguments to the parser.

after_pooling_forward(*gnn_layers*, *adj*, *x*, *concat=False*)

classmethod build_model_from_args(*args*)

forward(*batch*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

graph_classificatoin_loss(*batch*)

reset_parameters()

classmethod split_dataset(*dataset*, *args*)

training: bool

class cogdl.models.nn.gcnii.**GCNII**(*in_feats*, *hidden_size*, *out_feats*, *num_layers*, *dropout=0.5*, *alpha=0.1*, *lmbda=1*, *wd1=0.0*, *wd2=0.0*, *residual=False*, *actnn=False*)

Bases: `cogdl.models.base_model.BaseModel`

Implementation of GCNII in paper "Simple and Deep Graph Convolutional Networks".

Parameters

- **in_feats** (*int*) – Size of each input sample
- **hidden_size** (*int*) – Size of each hidden unit
- **out_feats** (*int*) – Size of each out sample
- **num_layers** (*int*) –
- **dropout** (*float*) –
- **alpha** (*float*) – Parameter of initial residual connection
- **lmbda** (*float*) – Parameter of identity mapping
- **wd1** (*float*) – Weight-decay for Fully-connected layers
- **wd2** (*float*) – Weight-decay for convolutional layers

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

get_optimizer(*args*)

predict(*graph*)

training: bool

class cogdl.models.nn.sign.**MLP**(*in_feats*, *out_feats*, *hidden_size*, *num_layers*, *dropout=0.0*, *activation='relu'*, *norm=None*, *act_first=False*, *bias=True*)

Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

predict(*data*)

training: bool

class cogdl.models.nn.mixhop.**MixHop**(*num_features*, *num_classes*, *dropout*, *layer1_pows*, *layer2_pows*)

Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

predict(*data*)

training: bool

class cogdl.models.nn.gat.**GAT**(*in_feats*, *hidden_size*, *out_features*, *num_layers*, *dropout*, *attn_drop*, *alpha*, *nhead*, *residual*, *last_nhead*, *norm=None*)

Bases: `cogdl.models.base_model.BaseModel`

The GAT model from the "Graph Attention Networks" paper

Parameters

- **num_features** (*int*) – Number of input features.
- **num_classes** (*int*) – Number of classes.
- **hidden_size** (*int*) – The dimension of node representation.
- **dropout** (*float*) – Dropout rate for model training.

- **alpha** (*float*) – Coefficient of leaky_relu.
- **nheads** (*int*) – Number of attention heads.

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*graph*)

training: bool

class cogdl.models.nn.han.**HAN**(*num_edge*, *w_in*, *w_out*, *num_class*, *num_nodes*, *num_layers*)
Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.nn.ppnp.**PPNP**(*nfeat*, *nhid*, *nclass*, *num_layers*, *dropout*, *propagation*, *alpha*, *niter*, *cache=True*)
Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*graph*)

training: bool

class cogdl.models.nn.grace.**GRACE**(*in_feats: int, hidden_size: int, proj_hidden_size: int, num_layers: int, drop_feature_rates: List[float], drop_edge_rates: List[float], tau: float = 0.5, activation: str = 'relu', batch_size: int = - 1*)

Bases: `cogdl.models.base_model.BaseModel`

static **add_args**(*parser*)
Add model-specific arguments to the parser.

classmethod **build_model_from_args**(*args*)

embed(*data*)

forward(*graph: cogdl.data.data.Graph, x: Optional[torch.Tensor] = None*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.nn.pprgo.**PPRGo**(*in_feats, hidden_size, out_feats, num_layers, alpha, dropout, activation='relu', nprop=2, norm='sym'*)

Bases: `cogdl.models.base_model.BaseModel`

static **add_args**(*parser*)
Add model-specific arguments to the parser.

classmethod **build_model_from_args**(*args*)

forward(*x, targets, ppr_scores*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*graph, batch_size=10000*)

training: bool

class cogdl.models.nn.gin.**GIN**(*num_layers, in_feats, out_feats, hidden_dim, num_mlp_layers, eps=0, pooling='sum', train_eps=False, dropout=0.5*)

Bases: `cogdl.models.base_model.BaseModel`

Graph Isomorphism Network from paper "How Powerful are Graph Neural Networks?".

Parameters

- **num_layers** – int Number of GIN layers
- **in_feats** – int Size of each input sample

- **out_feats** – int Size of each output sample
- **hidden_dim** – int Size of each hidden layer dimension
- **num_mlp_layers** – int Number of MLP layers
- **eps** – float32, optional Initial *epsilon* value, default: `0`
- **pooling** – str, optional Aggregator type to use, default:`sum`
- **train_eps** – bool, optional If True, *epsilon* will be a learnable parameter, default: `True`

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*batch*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

classmethod split_dataset(*dataset*, *args*)

training: bool

class cogdl.models.nn.grand.**Grand**(*nfeat*, *nhid*, *nclass*, *input_droprate*, *hidden_droprate*, *use_bn*, *dropnode_rate*, *order*, *alpha*)
Bases: `cogdl.models.base_model.BaseModel`

Implementation of GRAND in paper *"Graph Random Neural Networks for Semi-Supervised Learning on Graphs"* <https://arxiv.org/abs/2005.11079>

Parameters

- **nfeat** (*int*) – Size of each input features.
- **nhid** (*int*) – Size of hidden features.
- **nclass** (*int*) – Number of output classes.
- **input_droprate** (*float*) – Dropout rate of input features.
- **hidden_droprate** (*float*) – Dropout rate of hidden features.
- **use_bn** (*bool*) – Using batch normalization.
- **dropnode_rate** (*float*) – Rate of dropping elements of input features
- **tem** (*float*) – Temperature to sharpen predictions.
- **lam** (*float*) – Proportion of consistency loss of unlabelled data
- **order** (*int*) – Order of adjacency matrix
- **sample** (*int*) – Number of augmentations for consistency loss
- **alpha** (*float*) –

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

drop_node(*x*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

normalize_x(*x*)

predict(*data*)

rand_prop(*graph, x*)

training: bool

class cogdl.models.nn.gtn.**GTN**(*num_edge, num_channels, w_in, w_out, num_class, num_nodes, num_layers*)

Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

norm(*edge_index, num_nodes, edge_weight, improved=False, dtype=None*)

normalization(*H*)

training: bool

class cogdl.models.nn.rgcn.**LinkPredictRGCN**(*num_entities, num_rels, hidden_size, num_layers, regularizer='basis', num_bases=None, self_loop=True, sampling_rate=0.01, penalty=0, dropout=0.0, self_dropout=0.0*)

Bases: `cogdl.utils.link_prediction_utils.GNNLinkPredict`, `cogdl.models.base_model.BaseModel`

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

loss(*graph*, *scoring*)

predict(*graph*)

training: bool

class cogdl.models.nn.deepergcn.**DeeperGCN**(*in_feat*, *hidden_size*, *out_feat*, *num_layers*, *activation='relu'*, *dropout=0.0*, *aggr='max'*, *beta=1.0*, *p=1.0*, *learn_beta=False*, *learn_p=False*, *learn_msg_scale=True*, *use_msg_norm=False*, *edge_attr_size=None*)

Bases: `cogdl.models.base_model.BaseModel`

Implementation of DeeperGCN in paper "DeeperGCN: All You Need to Train Deeper GCNs"

Parameters

- **in_feat** (*int*) – the dimension of input features
- **hidden_size** (*int*) – the dimension of hidden representation
- **out_feat** (*int*) – the dimension of output features
- **num_layers** (*int*) – the number of layers
- **activation** (*str, optional*) – activation function. Defaults to "relu".
- **dropout** (*float, optional*) – dropout rate. Defaults to 0.0.
- **aggr** (*str, optional*) – aggregation function. Defaults to "max".
- **beta** (*float, optional*) – a coefficient for aggregation function. Defaults to 1.0.
- **p** (*float, optional*) – a coefficient for aggregation function. Defaults to 1.0.
- **learn_beta** (*bool, optional*) – whether beta is learnable. Defaults to False.
- **learn_p** (*bool, optional*) – whether p is learnable. Defaults to False.
- **learn_msg_scale** (*bool, optional*) – whether message scale is learnable. Defaults to True.
- **use_msg_norm** (*bool, optional*) – use message norm or not. Defaults to False.
- **edge_attr_size** (*int, optional*) – the dimension of edge features. Defaults to None.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*graph*)

training: bool

class cogdl.models.nn.drgat.**DrGAT**(*num_features*, *num_classes*, *hidden_size*, *num_heads*, *dropout*)

Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.models.nn.infograph.**InfoGraph**(*in_feats*, *hidden_dim*, *out_feats*, *num_layers=3*, *sup=False*)

Bases: `cogdl.models.base_model.BaseModel`

Implementation of Infograph in paper `"InfoGraph: Unsupervised and Semi-supervised Graph-Level Representation

Learning via Mutual Information Maximization" <https://openreview.net/forum?id=r1lfF2NYvH>__. `

in_feats [int] Size of each input sample.

out_feats [int] Size of each output sample.

num_layers [int, optional] Number of MLP layers in encoder, default: `3`.

unsup [bool, optional] Use unsupervised model if True, default: `True`.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*batch*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

reset_parameters()

classmethod split_dataset(*dataset*, *args*)

sup_forward(*batch*, *x*)

training: bool

unsup_forward(*batch*, *x*)

class cogdl.models.nn.dropedge_gcn.**DropEdge_GCN**(*nfeat, nhid, nclass, nhidlayer, dropout, baseblock, inputlayer, outputlayer, nbaselayer, activation, withbn, withloop, aggrmethod*)

Bases: `cogdl.models.base_model.BaseModel`

DropEdge: Towards Deep Graph Convolutional Networks on Node Classification Applying DropEdge to GCN @ https://arxiv.org/pdf/1907.10903.pdf

The model for the single kind of deepgcn blocks. The model architecture likes: inputlayer(nfeat)–block(nbaselayer, nhid)–. . . –outputlayer(nclass)–softmax(nclass)

|------ nhidlayer ----|

The total layer is nhidlayer*nbaselayer + 2. All options are configurable.

Args: Initial function. :param nfeat: the input feature dimension. :param nhid: the hidden feature dimension. :param nclass: the output feature dimension. :param nhidlayer: the number of hidden blocks. :param dropout: the dropout ratio. :param baseblock: the baseblock type, can be "mutigcn", "resgcn", "densegcn" and "inceptiongcn". :param inputlayer: the input layer type, can be "gcn", "dense", "none". :param outputlayer: the input layer type, can be "gcn", "dense". :param nbaselayer: the number of layers in one hidden block. :param activation: the activation function, default is ReLu. :param withbn: using batch normalization in graph convolution. :param withloop: using self feature modeling in graph convolution. :param aggrmethod: the aggregation function for baseblock, can be "concat" and "add". For "resgcn", the default

is "add", for others the default is "concat".

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

predict(*data*)

reset_parameters()

training: bool

class cogdl.models.nn.disengcn.**DisenGCN**(*in_feats, hidden_size, num_classes, K, iterations, tau, dropout, activation*)

Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*data*)

reset_parameters()

training: bool

class cogdl.models.nn.mlp.**MLP**(*in_feats*, *out_feats*, *hidden_size*, *num_layers*, *dropout=0.0*, *activation='relu'*, *norm=None*, *act_first=False*, *bias=True*)

Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*data*)

training: bool

class cogdl.models.nn.sgc.**sgc**(*in_feats*, *out_feats*)

Bases: *cogdl.models.base_model.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*data*)

training: bool

class cogdl.models.nn.sortpool.**SortPool**(*in_feats*, *hidden_dim*, *num_classes*, *num_layers*, *out_channel*, *kernel_size*, *k=30*, *dropout=0.5*)

Bases: *cogdl.models.base_model.BaseModel*

Implimentation of sortpooling in paper *"An End-to-End Deep Learning Architecture for Graph Classification" <https://www.cse.wustl.edu/~muhan/papers/AAAI_2018_DGCNN.pdf>__.*

Parameters

- **in_feats** (*int*) – Size of each input sample.
- **out_feats** (*int*) – Size of each output sample.
- **hidden_dim** (*int*) – Dimension of hidden layer embedding.
- **num_classes** (*int*) – Number of target classes.
- **num_layers** (*int*) – Number of graph neural network layers before pooling.
- **k** (*int, optional*) – Number of selected features to sort, default: `30`.
- **out_channel** (*int*) – Number of the first convolution's output channels.
- **kernel_size** (*int*) – Size of the first convolution's kernel.
- **dropout** (*float, optional*) – Size of dropout, default: `0.5`.

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*batch*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

classmethod split_dataset(*dataset, args*)

training: bool

class cogdl.models.nn.srgcn.**SRGCN**(*in_feats, hidden_size, out_feats, attention, activation, nhop, normalization, dropout, node_dropout, alpha, nhead, subheads*)
Bases: `cogdl.models.base_model.BaseModel`

static add_args(*parser*)
Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*data*)

training: bool

class cogdl.models.nn.unsup_graphsage.**SAGE**(*num_features*, *hidden_size*, *num_layers*, *sample_size*, *dropout*)

Bases: *cogdl.models.base_model.BaseModel*

Implementation of unsupervised GraphSAGE in paper *"Inductive Representation Learning on Large Graphs"* <https://cs.stanford.edu/people/jure/pubs/graphsage-nips17.pdf>

Parameters

- **num_features** (*int*) – Size of each input sample
- **hidden_size** (*int*) –
- **num_layers** (*int*) – The number of GNN layers.
- **samples_size** (*list*) – The number sampled neighbors of different orders
- **dropout** (*float*) –
- **walk_length** (*int*) – The length of random walk
- **negative_samples** (*int*) –

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

embed(*data*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

sampling(*edge_index*, *num_sample*)

training: bool

class cogdl.models.nn.daegc.**DAEGC**(*num_features*, *hidden_size*, *embedding_size*, *num_heads*, *dropout*, *num_clusters*)

Bases: *cogdl.models.base_model.BaseModel*

The DAEGC model from the "Attributed Graph Clustering: A Deep Attentional Embedding Approach" paper

Parameters

- **num_clusters** (*int*) – Number of clusters.
- **T** (*int*) – Number of iterations to recalculate P and Q
- **gamma** (*float*) – Hyperparameter that controls two parts of the loss.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*args*)

forward(*graph*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

get_2hop(*edge_index*)
add 2-hop neighbors as new edges

get_cluster_center()

get_features(*data*)

recon_loss(*z*, *adj*)

set_cluster_center(*center*)

training: bool

class cogdl.models.nn.agc.**AGC**(*num_clusters*, *max_iter*, *cpu*)
Bases: *cogdl.models.base_model.BaseModel*

The AGC model from the "Attributed Graph Clustering via Adaptive Graph Convolution" paper

Parameters

- **num_clusters** (*int*) – Number of clusters.
- **max_iter** (*int*) – Max iteration to increase k

static **add_args**(*parser*)
Add model-specific arguments to the parser.

classmethod **build_model_from_args**(*args*)

compute_intra(*x*, *clusters*)

forward(*data*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

2.10.4 Model Module

cogdl.models.**build_model**(*args*)

cogdl.models.**register_model**(*name*)
New model types can be added to cogdl with the *register_model()* function decorator. For example:

```
@register_model('gat')
class GAT(BaseModel):
    (...)
```

Parameters **name** (*str*) – the name of the model

cogdl.models.**try_adding_model_args**(*model*, *parser*)

2.11 data wrappers

2.11.1 Node Classification

class cogdl.wrappers.data_wrapper.node_classification.**ClusterWrapper**(*dataset*, *method='metis'*, *batch_size=20*, *n_cluster=100*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static **add_args**(*parser*)

get_train_dataset()

Return the *wrapped* dataset for specific usage. For example, return *ClusteredDataset* in cluster_dw for DDP training.

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_wrapper()

class cogdl.wrappers.data_wrapper.node_classification.**GraphSAGEDataWrapper**(*dataset*, *batch_size: int*, *sample_size: list*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static **add_args**(*parser*)

get_train_dataset()

Return the *wrapped* dataset for specific usage. For example, return *ClusteredDataset* in cluster_dw for DDP training.

test_wrapper()

train_transform(*batch*)

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_transform(*batch*)

val_wrapper()

class cogdl.wrappers.data_wrapper.node_classification.**M3SDataWrapper**(*dataset*, *label_rate*, *approximate*, *alpha*)

Bases: *cogdl.wrappers.data_wrapper.node_classification.node_classification_dw.FullBatchNodeClfDataWrapper*

static add_args(*parser*)

get_dataset()

post_stage(*stage*, *model_w_out*)
Processing after each run

pre_stage(*stage*, *model_w_out*)
Processing before each run

pre_transform()
Data Preprocessing before all runs

class cogdl.wrappers.data_wrapper.node_classification.**NetworkEmbeddingDataWrapper**(*dataset*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

class cogdl.wrappers.data_wrapper.node_classification.**FullBatchNodeClfDataWrapper**(*dataset*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

pre_transform()
Data Preprocessing before all runs

test_wrapper()

train_wrapper() → *cogdl.data.data.Graph*

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_wrapper()

class cogdl.wrappers.data_wrapper.node_classification.**PPRGoDataWrapper**(*dataset*, *topk*, *alpha=0.2*, *norm='sym'*, *batch_size=512*, *eps=0.0001*, *test_batch_size=- 1*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static **add_args**(*parser*)

test_wrapper()

train_wrapper()

batch: tuple(x, targets, ppr_scores, y) x: shape=(b, num_features) targets: shape=(num_edges_of_batch,)

ppr_scores: shape=(num_edges_of_batch,) y: shape=(b, num_classes)

val_wrapper()

class cogdl.wrappers.data_wrapper.node_classification.**SAGNDataWrapper**(*dataset*, *batch_size*, *label_nhop*, *threshold*, *nhop*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static **add_args**(*parser*)

post_stage_wrapper()

pre_stage(*stage*, *model_w_out*)
Processing before each run

pre_stage_transform(*batch*)

pre_transform()
Data Preprocessing before all runs

test_transform(*batch*)

test_wrapper()

train_transform(*batch*)

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_transform(*batch*)

val_wrapper()

2.11.2 Graph Classification

class cogdl.wrappers.data_wrapper.graph_classification.**GraphClassificationDataWrapper**(*dataset, degree_node_features=F, batch_size=32, train_ratio=0.5, test_ratio=0.3*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static add_args(*parser*)

setup_node_features()

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_wrapper()

class cogdl.wrappers.data_wrapper.graph_classification.**GraphEmbeddingDataWrapper**(*dataset, degree_node_features=False*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static add_args(*parser*)

pre_transform()

Data Preprocessing before all runs

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

class cogdl.wrappers.data_wrapper.graph_classification.**InfoGraphDataWrapper**(*dataset, degree_node_features=False, batch_size=32, train_ratio=0.5, test_ratio=0.3*)

Bases: *cogdl.wrappers.data_wrapper.graph_classification.graph_classification_dw.GraphClassificationDataWrapper*

test_wrapper()

class cogdl.wrappers.data_wrapper.graph_classification.**PATCHY_SAN_DataWrapper**(*dataset*, *num_sample*, *num_neighbor*, *stride*, **args*, ***kwargs*)

Bases: *cogdl.wrappers.data_wrapper.graph_classification.graph_classification_dw.GraphClassificationDataWrapper*

static add_args(*parser*)

pre_transform()
Data Preprocessing before all runs

2.11.3 Pretraining

class cogdl.wrappers.data_wrapper.pretraining.**GCCDataWrapper**(*dataset*, *batch_size*, *finetune=False*, *num_workers=4*, *rw_hops=64*, *subgraph_size=128*, *restart_prob=0.8*, *positional_embedding_size=128*, *task='node_classification'*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static add_args(*parser*)

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

2.11.4 Link Prediction

class cogdl.wrappers.data_wrapper.link_prediction.**EmbeddingLinkPredictionDataWrapper**(*dataset*, *negative_ratio*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

static add_args(*parser*)

pre_transform()
Data Preprocessing before all runs

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph

3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

class cogdl.wrappers.data_wrapper.link_prediction.**GNNKGLinkPredictionDataWrapper**(*dataset*)
Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_wrapper()

class cogdl.wrappers.data_wrapper.link_prediction.**GNNLinkPredictionDataWrapper**(*dataset*)
Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

pre_transform()
Data Preprocessing before all runs

test_wrapper()

static train_test_edge_split(*edge_index*, *num_nodes*, *val_ratio=0.1*, *test_ratio=0.2*)

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_wrapper()

2.11.5 Heterogeneous

class cogdl.wrappers.data_wrapper.heterogeneous.**HeterogeneousEmbeddingDataWrapper**(*dataset*)
Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

class cogdl.wrappers.data_wrapper.heterogeneous.**HeterogeneousGNNDataWrapper**(*dataset*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

val_wrapper()

class cogdl.wrappers.data_wrapper.heterogeneous.**MultiplexEmbeddingDataWrapper**(*dataset*)

Bases: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper

test_wrapper()

train_wrapper()

Returns

1. DataLoader
2. cogdl.Graph
3. list of DataLoader or Graph

Any other data formats other than DataLoader will not be traversed

2.12 model wrappers

2.12.1 Node Classification

class cogdl.wrappers.model_wrapper.node_classification.**DGIModelWrapper**(*model*, *optimizer_cfg*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.UnsupervisedModelWrapper

static add_args(*parser*)

static augment(*graph*)

setup_optimizer()

test_step(*graph*)

train_step(*subgraph*)

training: bool

class cogdl.wrappers.model_wrapper.node_classification.**GCNMixModelWrapper**(*model*, *optimizer_cfg*, *temperature*, *rampup_starts*, *rampup_ends*, *mixup_consistency*, *ema_decay*, *tau*, *k*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper`

GCNMixModelWrapper calls *forward_aux* in model *forward_aux* is similar to *forward* but ignores *spmm* operation.

static add_args(*parser*)

setup_optimizer()

test_step(*subgraph*)

train_step(*subgraph*)

training: bool

update_aux(*data*, *vector_labels*, *train_index*)

update_soft(*graph*)

val_step(*subgraph*)

class cogdl.wrappers.model_wrapper.node_classification.**GRACEModelWrapper**(*model*, *optimizer_cfg*, *tau*, *drop_feature_rates*, *drop_edge_rates*, *batch_fwd*, *proj_hidden_size*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.UnsupervisedModelWrapper`

static add_args(*parser*)

batched_loss(*z1: torch.Tensor*, *z2: torch.Tensor*, *batch_size: int*)

contrastive_loss(*z1: torch.Tensor*, *z2: torch.Tensor*)

prop(*graph: cogdl.data.data.Graph*, *x: torch.Tensor*, *drop_feature_rate: float = 0.0*, *drop_edge_rate: float = 0.0*)

setup_optimizer()

test_step(*graph*)

train_step(*subgraph*)

training: bool

class cogdl.wrappers.model_wrapper.node_classification.**GrandModelWrapper**(*model*, *optimizer_cfg*, *sample=2*, *temperature=0.5*, *lmbda=0.5*)

Bases: *cogdl.wrappers.model_wrapper.node_classification.node_classification_mw.NodeClfModelWrapper*

sample [int] Number of augmentations for consistency loss

temperature [float] Temperature to sharpen predictions.

lmbda [float] Proportion of consistency loss of unlabelled data

`static add_args`(*parser*)

`consistency_loss`(*logps*, *train_mask*)

`train_step`(*batch*)

`training: bool`

`class cogdl.wrappers.model_wrapper.node_classification.MVGRLModelWrapper`(*model*, *optimizer_cfg*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.UnsupervisedModelWrapper`

`setup_optimizer`()

`test_step`(*graph*)

`train_step`(*subgraph*)

`training: bool`

`class cogdl.wrappers.model_wrapper.node_classification.SelfAuxiliaryModelWrapper`(*model*, *optimizer_cfg*, *auxiliary_task*, *dropedge_rate*, *mask_ratio*, *sampling*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.UnsupervisedModelWrapper`

`static add_args`(*parser*)

`generate_virtual_labels`(*data*)

`pre_stage`(*stage*, *data_w*)

`setup_optimizer`()

`test_step`(*graph*)

`train_step`(*subgraph*)

`training: bool`

`class cogdl.wrappers.model_wrapper.node_classification.GraphSAGEModelWrapper`(*model*, *optimizer_cfg*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper`

`setup_optimizer`()

`test_step`(*batch*)

`train_step`(*batch*)

`training: bool`

`val_step`(*batch*)

class cogdl.wrappers.model_wrapper.node_classification.**UnsupGraphSAGEModelWrapper**(*model*, *optimizer_cfg*, *walk_length*, *negative_samples*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.UnsupervisedModelWrapper

static add_args(*parser*)

setup_optimizer()

test_step(*graph*)

train_step(*batch*)

training: bool

class cogdl.wrappers.model_wrapper.node_classification.**M3SModelWrapper**(*model*, *optimizer_cfg*, *n_cluster*, *num_new_labels*)

Bases: *cogdl.wrappers.model_wrapper.node_classification.node_classification_mw.NodeClfModelWrapper*

static add_args(*parser*)

pre_stage(*stage*, *data_w: cogdl.wrappers.data_wrapper.base_data_wrapper.DataWrapper*)

training: bool

class cogdl.wrappers.model_wrapper.node_classification.**NetworkEmbeddingModelWrapper**(*model*, *num_shuffle=1*, *training_percents=[0.1]*, *enhance=None*, *max_evals=10*, *num_workers=1*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.EmbeddingModelWrapper

static add_args(*parser*)

test_step(*batch*)

train_step(*batch*)

training: bool

class cogdl.wrappers.model_wrapper.node_classification.**NodeClfModelWrapper**(*model*, *optimizer_cfg*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper

set_early_stopping()

Returns

1. *str*, the monitoring metric
2. **tuple(*str*, *str*), that is, (the monitoring metric, *small* or *big*). The second parameter means,** *the smaller, the better* or *the bigger, the better*

setup_optimizer()

test_step(*batch*)

train_step(*subgraph*)

training: bool

val_step(*subgraph*)

class cogdl.wrappers.model_wrapper.node_classification.**CorrectSmoothModelWrapper**(*model*, *optimizer_cfg*)

Bases: *cogdl.wrappers.model_wrapper.node_classification.node_classification_mw.NodeClfModelWrapper*

static add_args(*parser*)

test_step(*batch*)

training: bool

val_step(*subgraph*)

class cogdl.wrappers.model_wrapper.node_classification.**PPRGoModelWrapper**(*model*, *optimizer_cfg*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper

setup_optimizer()

test_step(*batch*)

train_step(*batch*)

training: bool

val_step(*batch*)

class cogdl.wrappers.model_wrapper.node_classification.**SAGNModelWrapper**(*model*, *optimizer_cfg*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper

pre_stage(*stage*, *data_w*)

setup_optimizer()

test_step(*batch*)

train_step(*batch*)

training: bool

val_step(*batch*)

2.12.2 Graph Classification

class cogdl.wrappers.model_wrapper.graph_classification.**GraphClassificationModelWrapper**(*model*, *optimizer_cfg*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper

setup_optimizer()

test_step(*batch*)

train_step(*batch*)

training: bool

val_step(*batch*)

class cogdl.wrappers.model_wrapper.graph_classification.**GraphEmbeddingModelWrapper**(*model*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.EmbeddingModelWrapper`

test_step(*batch*)

train_step(*batch*)

training: bool

class cogdl.wrappers.model_wrapper.graph_classification.**InfoGraphModelWrapper**(*model*, *optimizer_cfg*, *sup=False*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper`

static **add_args**(*parser*)

static **mi_loss**(*pos_mask*, *neg_mask*, *mi*, *pos_div*, *neg_div*)

setup_optimizer()

sup_loss(*pred*, *batch*)

test_step(*dataset*)

train_step(*batch*)

training: bool

unsup_loss(*graph_feat*, *node_feat*, *batch*)

2.12.3 Pretraining

class cogdl.wrappers.model_wrapper.pretraining.**GCCModelWrapper**(*model*, *optimizer_cfg*, *nce_k*, *nce_t*, *momentum*, *output_size*, *finetune=False*, *num_classes=1*, *model_path='gcc_pretrain.pt'*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper`

static **add_args**(*parser*)

load_checkpoint(*path*)

post_stage(*stage*, *data_w*)

pre_stage(*stage*, *data_w*)

save_checkpoint(*path*)

setup_optimizer()

train_step(*batch*)

train_step_finetune(*batch*)

train_step_pretraining(*batch*)

training: bool

2.12.4 Link Prediction

class cogdl.wrappers.model_wrapper.link_prediction.**EmbeddingLinkPredictionModelWrapper**(*model*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.EmbeddingModelWrapper

test_step(*batch*)

train_step(*graph*)

training: bool

class cogdl.wrappers.model_wrapper.link_prediction.**GNNKGLinkPredictionModelWrapper**(*model*, *optimizer_cfg*, *score_func*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper

static **add_args**(*parser*)

eval_step(*graph*, *mask1*, *mask2*)

set_early_stopping()

Returns

1. *str*, the monitoring metric
2. **tuple(*str*, *str*), that is, (the monitoring metric, *small* or *big*). The second parameter means,** *the smaller, the better* or *the bigger, the better*

setup_optimizer()

test_step(*subgraph*)

train_step(*subgraph*)

training: bool

val_step(*subgraph*)

class cogdl.wrappers.model_wrapper.link_prediction.**GNNLinkPredictionModelWrapper**(*model*, *optimizer_cfg*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper

static **get_link_labels**(*num_pos*, *num_neg*, *device=None*)

set_early_stopping()

Returns

1. *str*, the monitoring metric
2. **tuple(*str*, *str*), that is, (the monitoring metric, *small* or *big*). The second parameter means,** *the smaller, the better* or *the bigger, the better*

setup_optimizer()

test_step(*subgraph*)

train_step(*subgraph*)

training: bool

val_step(*subgraph*)

2.12.5 Heterogeneous

class cogdl.wrappers.model_wrapper.heterogeneous.**HeterogeneousEmbeddingModelWrapper**(*model*, *hidden_size=200*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.EmbeddingModelWrapper

static add_args(*parser: argparse.ArgumentParser*)
Add task-specific arguments to the parser.

test_step(*batch*)

train_step(*batch*)

training: bool

class cogdl.wrappers.model_wrapper.heterogeneous.**HeterogeneousGNNModelWrapper**(*model*, *optimizer_cfg*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper

setup_optimizer()

test_step(*batch*)

train_step(*batch*)

training: bool

val_step(*batch*)

class cogdl.wrappers.model_wrapper.heterogeneous.**MultiplexEmbeddingModelWrapper**(*model*, *hidden_size=200*, *eval_type='all'*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.EmbeddingModelWrapper

static add_args(*parser: argparse.ArgumentParser*)
Add task-specific arguments to the parser.

test_step(*batch*)

train_step(*batch*)

training: bool

2.12.6 Clustering

class cogdl.wrappers.model_wrapper.clustering.**AGCModelWrapper**(*model*, *optimizer_cfg*, *num_clusters*, *cluster_method='kmeans'*, *evaluation='full'*, *max_iter=5*)

Bases: cogdl.wrappers.model_wrapper.base_model_wrapper.EmbeddingModelWrapper

static add_args(*parser*)

test_step(*batch*)

train_step(*graph*)

training: bool

class cogdl.wrappers.model_wrapper.clustering.**DAEGCModelWrapper**(*model*, *optimizer_cfg*, *num_clusters*, *cluster_method='kmeans'*, *evaluation='full'*, *T=5*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper`

static add_args(*parser*)

cluster_loss(*P*, *Q*)

getP(*Q*)

getQ(*z*, *cluster_center*)

post_stage(*stage*, *data_w*)

pre_stage(*stage*, *data_w*)

recon_loss(*z*, *adj*)

setup_optimizer()

test_step(*subgraph*)

train_step(*subgraph*)

training: bool

class cogdl.wrappers.model_wrapper.clustering.**GAEModelWrapper**(*model*, *optimizer_cfg*, *num_clusters*, *cluster_method='kmeans'*, *evaluation='full'*)

Bases: `cogdl.wrappers.model_wrapper.base_model_wrapper.ModelWrapper`

static add_args(*parser*)

pre_stage(*stage*, *data_w*)

setup_optimizer()

test_step(*subgraph*)

train_step(*subgraph*)

training: bool

2.13 layers

class cogdl.layers.gcn_layer.**GCNLayer**(*in_features*, *out_features*, *dropout=0.0*, *activation=None*, *residual=False*, *norm=None*, *bias=True*, ***kwargs*)

Bases: `torch.nn.modules.module.Module`

Simple GCN layer, similar to https://arxiv.org/abs/1609.02907

forward(*graph*, *x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

reset_parameters()

training: bool

class cogdl.layers.gat_layer.**GATLayer**(*in_feats*, *out_feats*, *nhead=1*, *alpha=0.2*, *attn_drop=0.5*, *activation=None*, *residual=False*, *norm=None*)

Bases: torch.nn.modules.module.Module

Sparse version GAT layer, similar to https://arxiv.org/abs/1710.10903

forward(*graph*, *x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

reset_parameters()

training: bool

class cogdl.layers.sage_layer.**MaxAggregator**

Bases: object

class cogdl.layers.sage_layer.**MeanAggregator**

Bases: object

class cogdl.layers.sage_layer.**SAGELayer**(*in_feats*, *out_feats*, *normalize=False*, *aggr='mean'*, *dropout=0.0*, *norm=None*, *activation=None*, *residual=False*)

Bases: torch.nn.modules.module.Module

forward(*graph*, *x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.layers.sage_layer.**SumAggregator**

Bases: object

class cogdl.layers.gin_layer.**GINLayer**(*apply_func=None*, *eps=0*, *train_eps=True*)

Bases: torch.nn.modules.module.Module

Graph Isomorphism Network layer from paper "How Powerful are Graph Neural Networks?".

$$h_i^{(l+1)} = f_\Theta\left((1+\epsilon)h_i^l + \mathrm{sum}\left(\left\{h_j^l, j \in \mathcal{N}(i)\right\}\right)\right)$$

Parameters

- **apply_func** (*callable layer function)*) – layer or function applied to update node feature
- **eps** (*float32, optional*) – Initial *epsilon* value.

- **train_eps** (*bool, optional*) – If True, *epsilon* will be a learnable parameter.

forward(*graph, x*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.layers.gcnii_layer.**GCNIILayer**(*n_channels, alpha=0.1, beta=1, residual=False*)
Bases: `torch.nn.modules.module.Module`

forward(*graph, x, init_x*)
Symmetric normalization

reset_parameters()

training: bool

class cogdl.layers.deepergcn_layer.**BondEncoder**(*bond_dim_list, emb_size*)
Bases: `torch.nn.modules.module.Module`

forward(*edge_attr*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.layers.deepergcn_layer.**EdgeEncoder**(*in_feats, out_feats, bias=False*)
Bases: `torch.nn.modules.module.Module`

forward(*edge_attr*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.layers.deepergcn_layer.**GENConv**(*in_feats: int, out_feats: int, aggr: str = 'softmax_sg', beta: float = 1.0, p: float = 1.0, learn_beta: bool = False, learn_p: bool = False, use_msg_norm: bool = False, learn_msg_scale: bool = True, norm: Optional[str] = None, residual: bool = False, activation: Optional[str] = None, num_mlp_layers: int = 2, edge_attr_size: Optional[list] = None*)

Bases: `torch.nn.modules.module.Module`

forward(*graph, x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

message_norm(*x, msg*)

training: bool

class cogdl.layers.deepergcn_layer.**ResGNNLayer**(*conv, in_channels, activation='relu', norm='batchnorm', dropout=0.0, out_norm=None, out_channels=- 1, residual=True, checkpoint_grad=False*)

Bases: `torch.nn.modules.module.Module`

Implementation of DeeperGCN in paper "DeeperGCN: All You Need to Train Deeper GCNs"

Parameters

- **conv** (*nn.Module*) – An instance of GNN Layer, recieving (graph, x) as inputs
- **n_channels** (*int*) – size of input features
- **activation** (*str*) –
- **norm** (*str*) – type of normalization, `batchnorm` as default
- **dropout** (*float*) –
- **checkpoint_grad** (*bool*) –

forward(*graph, x, dropout=None, *args, **kwargs*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.layers.disengcn_layer.**DisenGCNLayer**(*in_feats, out_feats, K, iterations, tau=1.0, activation='leaky_relu'*)

Bases: `torch.nn.modules.module.Module`

Implementation of "Disentangled Graph Convolutional Networks".

forward(*graph*, *x*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

reset_parameters()

training: bool

class cogdl.layers.han_layer.**AttentionLayer**(*num_features*)
Bases: `torch.nn.modules.module.Module`

forward(*x*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.layers.han_layer.**HANLayer**(*num_edge*, *w_in*, *w_out*)
Bases: `torch.nn.modules.module.Module`

forward(*graph*, *x*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.layers.mlp_layer.**MLP**(*in_feats*, *out_feats*, *hidden_size*, *num_layers*, *dropout=0.0*, *activation='relu'*, *norm=None*, *act_first=False*, *bias=True*)
Bases: `torch.nn.modules.module.Module`

Multilayer perception with normalization

$$x^{(i+1)} = \sigma(W^i x^{(i)})$$

Parameters

- **in_feats** (*int*) – Size of each input sample.
- **out_feats** (*int*) – Size of each output sample.
- **hidden_dim** (*int*) – Size of hidden layer dimension.
- **use_bn** (*bool, optional*) – Apply batch normalization if True, default: *True*.

forward(*x*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

reset_parameters()

training: bool

class cogdl.layers.pprgo_layer.**LinearLayer**(*in_features*, *out_features*, *bias=True*)
Bases: `torch.nn.modules.module.Module`

forward(*input*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

reset_parameters()

training: bool

class cogdl.layers.pprgo_layer.**PPRGoLayer**(*in_feats*, *hidden_size*, *out_feats*, *num_layers*, *dropout*, *activation='relu'*)
Bases: `torch.nn.modules.module.Module`

forward(*x*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

---

training: bool

class cogdl.layers.rgcn_layer.**RGCNLayer**(*in_feats*, *out_feats*, *num_edge_types*, *regularizer='basis'*, *num_bases=None*, *self_loop=True*, *dropout=0.0*, *self_dropout=0.0*, *layer_norm=True*, *bias=True*)
Bases: `torch.nn.modules.module.Module`

Implementation of Relational-GCN in paper "Modeling Relational Data with Graph Convolutional Networks"

Parameters

- **in_feats** (*int*) – Size of each input embedding.
- **out_feats** (*int*) – Size of each output embedding.
- **num_edge_type** (*int*) – The number of edge type in knowledge graph.

- **regularizer** (*str, optional*) – Regularizer used to avoid overfitting, `basis` or `bdd`, default : `basis`.
- **num_bases** (*int, optional*) – The number of basis, only used when *regularizer* is *basis*, default : `None`.
- **self_loop** (*bool, optional*) – Add self loop embedding if True, default : `True`.
- **dropout** (*float*) –
- **self_dropout** (*float, optional*) – Dropout rate of self loop embedding, default : `0.0`
- **layer_norm** (*bool, optional*) – Use layer normalization if True, default : `True`
- **bias** (*bool*) –

basis_forward(*graph, x*)

bdd_forward(*graph, x*)

forward(*graph, x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

reset_parameters()

training: bool

Modified from https://github.com/GraphSAINT/GraphSAINT

class cogdl.layers.saint_layer.**SAINTLayer**(*dim_in, dim_out, dropout=0.0, act='relu', order=1, aggr='mean', bias='norm-nn', **kwargs*)

Bases: `torch.nn.modules.module.Module`

forward(*graph, x*)

Inputs: graph normalized adj matrix of the subgraph x 2D matrix of input node features

Outputs: feat_out 2D matrix of output node features

training: bool

class cogdl.layers.sgc_layer.**SGCLayer**(*in_features, out_features, order=3*)

Bases: `torch.nn.modules.module.Module`

forward(*graph, x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.layers.mixhop_layer.**MixHopLayer**(*num_features*, *adj_pows*, *dim_per_pow*)

Bases: torch.nn.modules.module.Module

adj_pow_x(*graph*, *x*, *p*)

forward(*graph*, *x*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

reset_parameters()

training: bool

class cogdl.layers.se_layer.**SELayer**(*in_channels*, *se_channels*)

Bases: torch.nn.modules.module.Module

Squeeze-and-excitation networks

forward(*x*)

training: bool

2.14 options

cogdl.options.**add_data_wrapper_args**(*parser*)

cogdl.options.**add_dataset_args**(*parser*)

cogdl.options.**add_model_args**(*parser*)

cogdl.options.**add_model_wrapper_args**(*parser*)

cogdl.options.**get_default_args**(*dataset*, *model*, ***kwargs*)

cogdl.options.**get_diff_args**(*args1*, *args2*)

cogdl.options.**get_display_data_parser**()

cogdl.options.**get_download_data_parser**()

cogdl.options.**get_parser**()

cogdl.options.**get_training_parser**()

cogdl.options.**parse_args_and_arch**(*parser*, *args*)

2.15 utils

class cogdl.utils.utils.**ArgClass**
Bases: `object`

cogdl.utils.utils.**alias_draw**(*J*, *q*)
Draw sample from a non-uniform discrete distribution using alias sampling.

cogdl.utils.utils.**alias_setup**(*probs*)
Compute utility lists for non-uniform sampling from discrete distributions. Refer to https://hips.seas.harvard.edu/blog/2013/03/03/the-alias-method-efficient-sampling-with-many-discrete-outcomes/ for details

cogdl.utils.utils.**batch_max_pooling**(*x*, *batch*)

cogdl.utils.utils.**batch_mean_pooling**(*x*, *batch*)

cogdl.utils.utils.**batch_sum_pooling**(*x*, *batch*)

cogdl.utils.utils.**build_args_from_dict**(*dic*)

cogdl.utils.utils.**cycle_index**(*num*, *shift*)

cogdl.utils.utils.**download_url**(*url*, *folder*, *name=None*, *log=True*)
Downloads the content of an URL to a specific folder.

Parameters

- **url** (*string*) – The url.
- **folder** (*string*) – The folder.
- **name** (*string*) – saved filename.
- **log** (*bool, optional*) – If `False`, will not print anything to the console. (default: `True`)

cogdl.utils.utils.**get_activation**(*act: str*, *inplace=False*)

cogdl.utils.utils.**get_memory_usage**(*print_info=False*)
Get accurate gpu memory usage by querying torch runtime

cogdl.utils.utils.**get_norm_layer**(*norm: str*, *channels: int*)

Parameters

- **norm** – str type of normalization: *layernorm*, *batchnorm*, *instancenorm*
- **channels** – int size of features for normalization

cogdl.utils.utils.**identity_act**(*input*)

cogdl.utils.utils.**makedirs**(*path*)

cogdl.utils.utils.**print_result**(*results*, *datasets*, *model_name*)

cogdl.utils.utils.**set_random_seed**(*seed*)

cogdl.utils.utils.**split_dataset_general**(*dataset*, *args*)

cogdl.utils.utils.**tabulate_results**(*results_dict*)

cogdl.utils.utils.**untar**(*path*, *fname*, *deleteTar=True*)
Unpacks the given archive file to the same directory, then (by default) deletes the archive file.

cogdl.utils.utils.**update_args_from_dict**(*args*, *dic*)

class cogdl.utils.evaluator.**Accuracy**(*mini_batch=False*)
Bases: object

clear()

evaluate()

class cogdl.utils.evaluator.**BCEWithLogitsLoss**
Bases: torch.nn.modules.module.Module

training: bool

class cogdl.utils.evaluator.**BaseEvaluator**(*eval_func*)
Bases: object

clear()

evaluate()

class cogdl.utils.evaluator.**CrossEntropyLoss**
Bases: torch.nn.modules.module.Module

training: bool

class cogdl.utils.evaluator.**MultiClassMicroF1**(*mini_batch=False*)
Bases: *cogdl.utils.evaluator.Accuracy*

class cogdl.utils.evaluator.**MultiLabelMicroF1**(*mini_batch=False*)
Bases: *cogdl.utils.evaluator.Accuracy*

cogdl.utils.evaluator.**accuracy**(*y_pred*, *y_true*)

cogdl.utils.evaluator.**bce_with_logits_loss**(*y_pred*, *y_true*, *reduction='mean'*)

cogdl.utils.evaluator.**cross_entropy_loss**(*y_pred*, *y_true*)

cogdl.utils.evaluator.**multiclass_f1**(*y_pred*, *y_true*)

cogdl.utils.evaluator.**multilabel_f1**(*y_pred*, *y_true*, *sigmoid=False*)

cogdl.utils.evaluator.**setup_evaluator**(*metric: Union[str, Callable]*)

class cogdl.utils.sampling.**RandomWalker**(*adj=None*, *num_nodes=None*)
Bases: object

build_up(*adj*, *num_nodes*)

walk(*start*, *walk_length*, *restart_p=0.0*)

cogdl.utils.sampling.**random_walk**(*start*, *length*, *indptr*, *indices*, *p=0.0*)

Parameters

- **start** – np.array(dtype=np.int32)
- **length** – int
- **indptr** – np.array(dtype=np.int32)
- **indices** – np.array(dtype=np.int32)
- **p** – float

Returns list(np.array(dtype=np.int32))

cogdl.utils.graph_utils.**add_remaining_self_loops**(*edge_index*, *edge_weight=None*, *fill_value=1*, *num_nodes=None*) cogdl.utils.graph_utils.**add_self_loops**(*edge_index*, *edge_weight=None*, *fill_value=1*, *num_nodes=None*)

cogdl.utils.graph_utils.**coalesce**(*row*, *col*, *value=None*)

cogdl.utils.graph_utils.**coo2csc**(*row*, *col*, *data*, *num_nodes=None*, *sorted=False*)

cogdl.utils.graph_utils.**coo2csr**(*row*, *col*, *data*, *num_nodes=None*, *ordered=False*)

cogdl.utils.graph_utils.**coo2csr_index**(*row*, *col*, *num_nodes=None*)

cogdl.utils.graph_utils.**csr2coo**(*indptr*, *indices*, *data*)

cogdl.utils.graph_utils.**csr2csc**(*indptr*, *indices*, *data=None*)

cogdl.utils.graph_utils.**get_degrees**(*row*, *col*, *num_nodes=None*)

cogdl.utils.graph_utils.**negative_edge_sampling**(*edge_index: Union[Tuple, torch.Tensor]*, *num_nodes: Optional[int] = None*, *num_neg_samples: Optional[int] = None*, *undirected: bool = False*)

cogdl.utils.graph_utils.**remove_self_loops**(*indices*, *values=None*)

cogdl.utils.graph_utils.**row_normalization**(*num_nodes*, *row*, *col*, *val=None*)

cogdl.utils.graph_utils.**sorted_coo2csr**(*row*, *col*, *data*, *num_nodes=None*, *return_index=False*)

cogdl.utils.graph_utils.**symmetric_normalization**(*num_nodes*, *row*, *col*, *val=None*)

cogdl.utils.graph_utils.**to_undirected**(*edge_index*, *num_nodes=None*)

Converts the graph given by `edge_index` to an undirected graph, so that $(j, i) \in \mathcal{E}$ for every edge $(i, j) \in \mathcal{E}$.

Parameters

- **edge_index** (*LongTensor*) – The edge indices.
- **num_nodes** (*int, optional*) – The number of nodes, *i.e.* `max_val + 1` of `edge_index`. (default: `None`)

Return type `LongTensor`

class cogdl.utils.link_prediction_utils.**ConvELayer**(*dim*, *num_filter=20*, *kernel_size=7*, *k_w=10*, *dropout=0.3*)

Bases: `torch.nn.modules.module.Module`

concat(*ent*, *rel*)

forward(*sub_emb*, *obj_emb*, *rel_emb*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*sub_emb*, *obj_emb*, *rel_emb*)

training: bool

class cogdl.utils.link_prediction_utils.**DistMultLayer**

Bases: `torch.nn.modules.module.Module`

forward(*sub_emb*, *obj_emb*, *rel_emb*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

predict(*sub_emb*, *obj_emb*, *rel_emb*)

training: bool

class cogdl.utils.link_prediction_utils.**GNNLinkPredict**
Bases: `torch.nn.modules.module.Module`

forward(*graph*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

get_edge_set(*edge_index*, *edge_types*)

training: bool

cogdl.utils.link_prediction_utils.**cal_mrr**(*embedding*, *rel_embedding*, *edge_index*, *edge_type*, *scoring*, *protocol='raw'*, *batch_size=1000*, *hits=[]*)

cogdl.utils.link_prediction_utils.**get_filtered_rank**(*heads*, *tails*, *rels*, *embedding*, *rel_embedding*, *batch_size*, *seen_data*)

cogdl.utils.link_prediction_utils.**get_rank**(*scores*, *target*)

cogdl.utils.link_prediction_utils.**get_raw_rank**(*heads*, *tails*, *rels*, *embedding*, *rel_embedding*, *batch_size*, *scoring*)

cogdl.utils.link_prediction_utils.**sampling_edge_uniform**(*edge_index*, *edge_types*, *edge_set*, *sampling_rate*, *num_rels*, *label_smoothing=0.0*, *num_entities=1*)

Parameters

- **edge_index** – edge index of graph
- **edge_types** –
- **edge_set** – set of all edges of the graph, (h, t, r)
- **sampling_rate** –
- **num_rels** –
- **label_smoothing** (*Optional*) –
- **num_entities** (*Optional*) –

Returns sampled existing edges rels: types of smapled existing edges sampled_edges_all: existing edges with corrupted edges sampled_types_all: types of existing and corrupted edges labels: 0/1

Return type sampled_edges

cogdl.utils.ppr_utils.**build_topk_ppr_matrix_from_data**(*edge_index*, **args*, ***kwargs*)

cogdl.utils.ppr_utils.**calc_ppr_topk_parallel**(*indptr*, *indices*, *deg*, *alpha*, *epsilon*, *nodes*, *topk*)

cogdl.utils.ppr_utils.**construct_sparse**(*neighbors*, *weights*, *shape*)

cogdl.utils.ppr_utils.**ppr_topk**(*adj_matrix*, *alpha*, *epsilon*, *nodes*, *topk*)
Calculate the PPR matrix approximately using Anderson.

cogdl.utils.ppr_utils.**topk_ppr_matrix**(*adj_matrix*, *alpha*, *eps*, *idx*, *topk*, *normalization='row'*)
Create a sparse matrix where each node has up to the topk PPR neighbors and their weights.

class cogdl.utils.prone_utils.**Gaussian**(*mu=0.5*, *theta=1*, *rescale=False*, *k=3*)
Bases: object

prop(*mx*, *emb*)

class cogdl.utils.prone_utils.**HeatKernel**(*t=0.5*, *theta0=0.6*, *theta1=0.4*)
Bases: object

prop(*mx*, *emb*)

prop_adjacency(*mx*)

class cogdl.utils.prone_utils.**HeatKernelApproximation**(*t=0.2*, *k=5*)
Bases: object

chebyshev(*mx*, *emb*)

prop(*mx*, *emb*)

taylor(*mx*, *emb*)

class cogdl.utils.prone_utils.**NodeAdaptiveEncoder**
Bases: object

- shrink negative values in signal/feature matrix
- no learning

static prop(*signal*)

class cogdl.utils.prone_utils.**PPR**(*alpha=0.5*, *k=10*)
Bases: object

applying sparsification to accelerate computation

prop(*mx*, *emb*)

class cogdl.utils.prone_utils.**ProNE**
Bases: object

class cogdl.utils.prone_utils.**SignalRescaling**
Bases: object

- **rescale signal of each node according to the degree of the node:**
  - sigmoid(degree)
  - sigmoid(1/degree)

prop(*mx*, *emb*)

cogdl.utils.prone_utils.**get_embedding_dense**(*matrix*, *dimension*)

cogdl.utils.prone_utils.**propagate**(*mx*, *emb*, *stype*, *space=None*) class cogdl.utils.srgcn_utils.**ColumnUniform**

Bases: `torch.nn.modules.module.Module`

forward(*edge_index*, *edge_attr*, *N*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**EdgeAttention**(*in_feat*)

Bases: `torch.nn.modules.module.Module`

forward(*x*, *edge_index*, *edge_attr*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**Gaussian**(*in_feat*)

Bases: `torch.nn.modules.module.Module`

forward(*x*, *edge_index*, *edge_attr*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**HeatKernel**(*in_feat*)

Bases: `torch.nn.modules.module.Module`

forward(*x*, *edge_index*, *edge_attr*)

Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the `Module` instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**Identity**(*in_feat*)
Bases: torch.nn.modules.module.Module

forward(*x*, *edge_index*, *edge_attr*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**NodeAttention**(*in_feat*)
Bases: torch.nn.modules.module.Module

forward(*x*, *edge_index*, *edge_attr*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**NormIdentity**
Bases: torch.nn.modules.module.Module

forward(*edge_index*, *edge_attr*, *N*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**PPR**(*in_feat*)
Bases: torch.nn.modules.module.Module

forward(*x*, *edge_index*, *edge_attr*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**RowSoftmax**
Bases: torch.nn.modules.module.Module

forward(*edge_index*, *edge_attr*, *N*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**RowUniform**
Bases: torch.nn.modules.module.Module

forward(*edge_index*, *edge_attr*, *N*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

class cogdl.utils.srgcn_utils.**SymmetryNorm**
Bases: torch.nn.modules.module.Module

forward(*edge_index*, *edge_attr*, *N*)
Defines the computation performed at every call.

Should be overridden by all subclasses.

Note: Although the recipe for forward pass needs to be defined within this function, one should call the Module instance afterwards instead of this since the former takes care of running the registered hooks while the latter silently ignores them.

training: bool

cogdl.utils.srgcn_utils.**act_attention**(*attn_type*)

cogdl.utils.srgcn_utils.**act_map**(*act*)

cogdl.utils.srgcn_utils.**act_normalization**(*norm_type*)

2.16 experiments

class cogdl.experiments.**AutoML**(*args*)

Bases: object

Parameters **search_space** – function to obtain hyper-parameters to search

run()

cogdl.experiments.**auto_experiment**(*args*)

cogdl.experiments.**default_search_space**(*trial*)

cogdl.experiments.**experiment**(*dataset*, *model=None*, ***kwargs*)

cogdl.experiments.**gen_variants**(***items*)

cogdl.experiments.**getpid**(_)

cogdl.experiments.**output_results**(*results_dict*, *tablefmt='github'*)

cogdl.experiments.**raw_experiment**(*args*)

cogdl.experiments.**set_best_config**(*args*)

cogdl.experiments.**train**(*args*)

cogdl.experiments.**train_parallel**(*args*)

cogdl.experiments.**variant_args_generator**(*args*, *variants*)

Form variants as group with size of num_workers

2.17 pipelines

class cogdl.pipelines.**DatasetPipeline**(*app: str*, ***kwargs*)

Bases: *cogdl.pipelines.Pipeline*

class cogdl.pipelines.**DatasetStatsPipeline**(*app: str*, ***kwargs*)

Bases: *cogdl.pipelines.DatasetPipeline*

class cogdl.pipelines.**DatasetVisualPipeline**(*app: str*, ***kwargs*)

Bases: *cogdl.pipelines.DatasetPipeline*

class cogdl.pipelines.**GenerateEmbeddingPipeline**(*app: str*, *model: str*, ***kwargs*)

Bases: *cogdl.pipelines.Pipeline*

class cogdl.pipelines.**OAGBertInferencePipepline**(*app: str*, *model: str*, ***kwargs*)

Bases: *cogdl.pipelines.Pipeline*

class cogdl.pipelines.**Pipeline**(*app: str*, ***kwargs*)

Bases: object

class cogdl.pipelines.**RecommendationPipepline**(*app: str*, *model: str*, ***kwargs*)

Bases: *cogdl.pipelines.Pipeline*

cogdl.pipelines.**check_app**(*app: str*)

cogdl.pipelines.**pipeline**(*app: str*, ***kwargs*) → *cogdl.pipelines.Pipeline*

CHAPTER

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