CogDL Documentation

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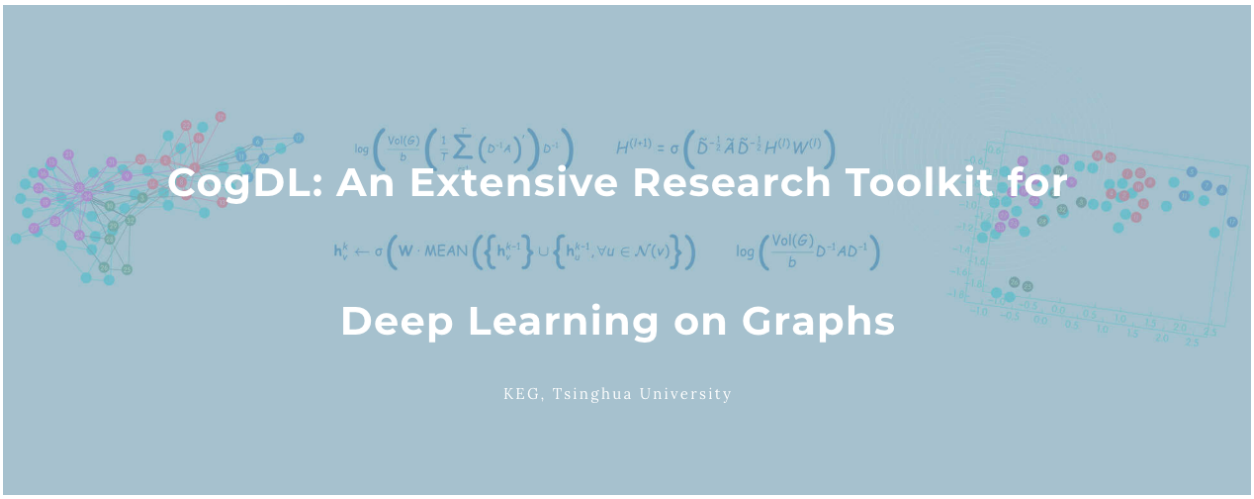

CogDL is a graph representation learning toolkit that allows researchers and developers to easily train and compare baseline or custom models for node classification, link prediction and other tasks on graphs. It provides implementations of many popular models, including: non-GNN Baselines like Deepwalk, LINE, NetMF, GNN Baselines like GCN, GAT, GraphSAGE.

CogDL provides these features:

- Task-Oriented: CogDL focuses on tasks on graphs and provides corresponding models, datasets, and leaderboards.
- Easy-Running: CogDL supports running multiple experiments simultaneously on multiple models and datasets under a specific task using multiple GPUs.
- Multiple Tasks: CogDL supports node classification and link prediction tasks on homogeneous/heterogeneous networks, as well as graph classification.
- Extensibility: You can easily add new datasets, models and tasks and conduct experiments for them!
- Supported tasks:
  - Node classification
  - Link prediction
  - Graph classification
  - Community detection (testing)
  - Social influence prediction (testing)
  - Graph reasoning (todo)
  - Graph pre-training (todo)
  - Combinatorial optimization on graphs (todo)

CHAPTER

ONE

INSTALL

- PyTorch version >= 1.0.0
- Python version >= 3.6
- PyTorch Geometric (optional)

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

Please follow the instructions here to install PyTorch Geometric: https://github.com/rusty1s/pytorch_geometric/#installation.

Install other dependencies:

```
>>> pip install -e .
```

CHAPTER

TWO

TUTORIAL

This guide can help you start working with CogDL.

2.1 Create a model

Here, we will create a spectral clustering model, which is a very simple graph embedding algorithm. We name it spectral.py and put it in cogdl/models/emb directory.

First we import necessary library like numpy, scipy, networkx, sklearn, we also import API like 'BaseModel' and 'register_model' from cogl/models/ to build our new model:

```
import numpy as np
import networkx as nx
import scipy.sparse as sp
from sklearn import preprocessing
from .. import BaseModel, register_model
```

Then we use function decorator to declare new model for CogDL

```
@register_model('spectral')
class Spectral(BaseModel):
    (...)
```

We have to implement method 'build_model_from_args' in spectral.py. If it need more parameters to train, we can use 'add_args' to add model-specific arguments.

```
@staticmethod
def add_args(parser):
    """Add model-specific arguments to the parser."""
    pass

@classmethod
def build_model_from_args(cls, args):
    return cls(args.hidden_size)

def __init__(self, dimension):
    super(Spectral, self).__init__()
    self.dimension = dimension
```

Each new model should provide a 'train' method to obtain representation.

```
def train(self, G):
    matrix = nx.normalized_laplacian_matrix(G).todense()
    matrix = np.eye(matrix.shape[0]) - np.asarray(matrix)
    ut, s, _ = sp.linalg.svds(matrix, self.dimension)
    emb_matrix = ut * np.sqrt(s)
    emb_matrix = preprocessing.normalize(emb_matrix, "l2")
    return emb_matrix
```

2.2 Create a dataset

In order to add a dataset into CogDL, you should know your dataset's format. We have provided several graph format like edgelist, matlab_matrix and pyg. If your dataset is same as the 'ppi' dataset, which contains two matrices: 'network' and 'group', you can register your dataset directly use above code.

```
@register_dataset("ppi")
class PPIDataset(MatlabMatrix):
    def __init__(self):
        dataset, filename = "ppi", "Homo_sapiens"
        url = "http://snap.stanford.edu/node2vec/"
        path = osp.join(osp.dirname(osp.realpath(__file__)), "../..", "data", dataset)
        super(PPIDataset, self).__init__(path, filename, url)
```

You should declare the name of the dataset, the name of file and the url, where our script can download resource.

2.3 Create a task

In order to evaluate some methods on several datasets, we can build a task and evaluate learned representation. The BaseTask class are:

```
class BaseTask(object):
    @staticmethod
    def add_args(parser):
        """Add task-specific arguments to the parser."""
        pass

    def __init__(self, args):
        pass

    def train(self, num_epoch):
        raise NotImplementedError
```

we can create a subclass to implement 'train' method like CommunityDetection, which get representation of each node and apply clustering algorithm(K-means) to evaluate.

```
@register_task("community_detection")
class CommunityDetection(BaseTask):
    """Community Detection task."""

    @staticmethod
    def add_args(parser):
        """Add task-specific arguments to the parser."""
        parser.add_argument("--hidden-size", type=int, default=128)
```

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```
        parser.add_argument("--num-shuffle", type=int, default=5)

    def __init__(self, args):
        super(CommunityDetection, self).__init__(args)
        dataset = build_dataset(args)
        self.data = dataset[0]

        self.num_nodes, self.num_classes = self.data.y.shape
        self.label = np.argmax(self.data.y, axis=1)
        self.model = build_model(args)
        self.hidden_size = args.hidden_size
        self.num_shuffle = args.num_shuffle

    def train(self):
        G = nx.Graph()
        G.add_edges_from(self.data.edge_index.t().tolist())
        embeddings = self.model.train(G)

        clusters = [30, 50, 70]
        all_results = defaultdict(list)
        for num_cluster in clusters:
            for _ in range(self.num_shuffle):
                model = KMeans(n_clusters=num_cluster).fit(embeddings)
                nmi_score = normalized_mutual_info_score(self.label, model.labels_)
                all_results[num_cluster].append(nmi_score)

        return dict(
            (
                f"normalized_mutual_info_score {num_cluster}",
                sum(all_results[num_cluster]) / len(all_results[num_cluster]),
            )
            for num_cluster in sorted(all_results.keys())
        )
```

2.4 Combine model, dataset and task

After create your model, dataset and task, we could combine them together to learn representation from a model on a dataset and evaluate its performance according to a task. We use 'build_model', 'build_dataset', 'build_task' method to build them with cooresponding parameters.

```
from cogdl.tasks import build_task
from cogdl.datasets import build_dataset
from cogdl.models import build_model
from cogdl.utils import build_args_from_dict

def test_deepwalk_ppi():
    default_dict = {'hidden_size': 64, 'num_shuffle': 1, 'cpu': True}
    args = build_args_from_dict(default_dict)

    # model, dataset and task parameters
    args.model = 'spectral'
    args.dataset = 'ppi'
    args.task = 'community_detection'
```

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```
    # build model, dataset and task
    dataset = build_dataset(args)
    model = build_model(args)
    task = build_task(args)

    # train model and get evaluate results
    ret = task.train()
    print(ret)
```

CHAPTER

THREE

TASKS

3.1 Node Classification

In this tutorial, we will introduce a important task, node classification. In this task, we train a GNN model with partial node labels and use accuracy to measure the performance.

First we define the *NodeClassification* class.

```
@register_task("node_classification")
class NodeClassification(BaseTask):
    """Node classification task."""

    @staticmethod
    def add_args(parser):
        """Add task-specific arguments to the parser."""

    def __init__(self, args):
        super(NodeClassification, self).__init__(args)
```

Then we can build dataset according to args.

```
self.device = torch.device('cpu' if args.cpu else 'cuda')
dataset = build_dataset(args)
self.data = dataset.data
self.data.apply(lambda x: x.to(self.device))
args.num_features = dataset.num_features
args.num_classes = dataset.num_classes
```

After that, we can build model and use *Adam* to optimize the model.

```
model = build_model(args)
self.model = model.to(self.device)
self.patience = args.patience
self.max_epoch = args.max_epoch
self.optimizer = torch.optim.Adam(
    self.model.parameters(), lr=args.lr, weight_decay=args.weight_decay
)
```

We provide a training loop for node classification task. For each epoch, we first call *_train_step* to optimize our model and then call *_test_step* to compute the accuracy and loss.

```
def train(self):
    epoch_iter = tqdm(range(self.max_epoch))
    patience = 0
```

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```
    best_score = 0
    best_loss = np.inf
    max_score = 0
    min_loss = np.inf
    for epoch in epoch_iter:
        self._train_step()
        train_acc, _ = self._test_step(split="train")
        val_acc, val_loss = self._test_step(split="val")
        epoch_iter.set_description(
            f"Epoch: {epoch:03d}, Train: {train_acc:.4f}, Val: {val_acc:.4f}"
        )
        if val_loss <= min_loss or val_acc >= max_score:
            if val_loss <= best_loss:  # and val_acc >= best_score:
                best_loss = val_loss
                best_score = val_acc
                best_model = copy.deepcopy(self.model)
            min_loss = np.min((min_loss, val_loss))
            max_score = np.max((max_score, val_acc))
            patience = 0
        else:
            patience += 1
            if patience == self.patience:
                self.model = best_model
                epoch_iter.close()
                break

def _train_step(self):
    self.model.train()
    self.optimizer.zero_grad()
    self.model.loss(self.data).backward()
    self.optimizer.step()

def _test_step(self, split="val"):
    self.model.eval()
    logits = self.model.predict(self.data)
    _, mask = list(self.data(f"{split}_mask"))[0]
    loss = F.nll_loss(logits[mask], self.data.y[mask])

    pred = logits[mask].max(1)[1]
    acc = pred.eq(self.data.y[mask]).sum().item() / mask.sum().item()
    return acc, loss
```

Finally, we compute the accuracy scores of test set for the trained model.

```
test_acc, _ = self._test_step(split="test")
print(f"Test accuracy = {test_acc}")
return dict(Acc=test_acc)
```

The overall implementation of *NodeClassification* is at (https://github.com/THUDM/cogdl/blob/master/cogdl/tasks/node_classification.py).

To run NodeClassification, we can use the following command:

```
python scripts/train.py --task node_classification --dataset cora citeseer --model␣
↪pyg_gcn pyg_gat --seed 0 1 --max-epoch 500
```

Then We get experimental results like this:

Variant	Acc
('cora', 'pyg_gcn')	0.7785±0.0165
('cora', 'pyg_gat')	0.7925±0.0045
('citeseer', 'pyg_gcn')	0.6535±0.0195
('citeseer', 'pyg_gat')	0.6675±0.0025

3.2 Unsupervised Node Classification

In this tutorial, we will introduce a important task, unsupervised node classification. In this task, we usually apply L2 normalized logisitic regression to train a classifier and use F1-score to measure the performance.

First we define the *UnsupervisedNodeClassification* class, which has two parameters *hidden-size* and *num-shuffle* . *hidden-size* represents the dimension of node representation, while *num-shuffle* means the shuffle times in classifier.

```
@register_task("unsupervised_node_classification")
class UnsupervisedNodeClassification(BaseTask):
    """Node classification task."""

    @staticmethod
    def add_args(parser):
        """Add task-specific arguments to the parser."""
        # fmt: off
        parser.add_argument("--hidden-size", type=int, default=128)
        parser.add_argument("--num-shuffle", type=int, default=5)
        # fmt: on

    def __init__(self, args):
        super(UnsupervisedNodeClassification, self).__init__(args)
```

Then we can build dataset according to input graph's type, and get *self.label_matrix*.

```
dataset = build_dataset(args)
self.data = dataset[0]
if issubclass(dataset.__class__.__bases__[0], InMemoryDataset):
    self.num_nodes = self.data.y.shape[0]
    self.num_classes = dataset.num_classes
    self.label_matrix = np.zeros((self.num_nodes, self.num_classes), dtype=int)
    self.label_matrix[range(self.num_nodes), self.data.y] = 1
    self.data.edge_attr = self.data.edge_attr.t()
else:
    self.label_matrix = self.data.y
    self.num_nodes, self.num_classes = self.data.y.shape
```

After that, we can build model and run *model.train(G)* to obtain node representation.

```
self.model = build_model(args)
self.model_name = args.model
self.hidden_size = args.hidden_size
self.num_shuffle = args.num_shuffle
self.save_dir = args.save_dir
self.enhance = args.enhance
self.args = args
self.is_weighted = self.data.edge_attr is not None
```

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```
def train(self):
    G = nx.Graph()
    if self.is_weighted:
        edges, weight = (
            self.data.edge_index.t().tolist(),
            self.data.edge_attr.tolist(),
        )
        G.add_weighted_edges_from(
            [(edges[i][0], edges[i][1], weight[0][i]) for i in range(len(edges))]
        )
    else:
        G.add_edges_from(self.data.edge_index.t().tolist())
    embeddings = self.model.train(G)
```

The spectral propagation in ProNE can improve the quality of representation learned from other methods, so we can use *enhance_emb* to enhance performance.

```
    if self.enhance is True:
        embeddings = self.enhance_emb(G, embeddings)

def enhance_emb(self, G, embs):
    A = sp.csr_matrix(nx.adjacency_matrix(G))
    self.args.model = 'prone'
    self.args.step, self.args.theta, self.args.mu = 5, 0.5, 0.2
    model = build_model(self.args)
    embs = model._chebyshev_gaussian(A, embs)
    return embs
```

When the embeddings are obtained, we can save them at *self.save_dir*.

```
# Map node2id
    features_matrix = np.zeros((self.num_nodes, self.hidden_size))
    for vid, node in enumerate(G.nodes()):
        features_matrix[node] = embeddings[vid]

self.save_emb(features_matrix)

def save_emb(self, embs):
    name = os.path.join(self.save_dir, self.model_name + '_emb.npy')
    np.save(name, embs)
```

At last, we evaluate embedding via run *num_shuffle* times classification under different training ratio with *features_matrix* and *label_matrix*.

```
return self._evaluate(features_matrix, label_matrix, self.num_shuffle)

    def _evaluate(self, features_matrix, label_matrix, num_shuffle):
        # shuffle, to create train/test groups
        shuffles = []
        for _ in range(num_shuffle):
            shuffles.append(skshuffle(features_matrix, label_matrix))

        # score each train/test group
        all_results = defaultdict(list)
        training_percents = [0.1, 0.3, 0.5, 0.7, 0.9]
```

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```
        for train_percent in training_percents:
            for shuf in shuffles:
```

In each shuffle, split data into two parts(training and testing) and use *LogisticRegression* to evaluate.

```
X, y = shuf

training_size = int(train_percent * self.num_nodes)

X_train = X[:training_size, :]
y_train = y[:training_size, :]

X_test = X[training_size:, :]
y_test = y[training_size:, :]

clf = TopKRanker(LogisticRegression())
clf.fit(X_train, y_train)

# find out how many labels should be predicted
top_k_list = list(map(int, y_test.sum(axis=1).T.tolist()[0]))
preds = clf.predict(X_test, top_k_list)
result = f1_score(y_test, preds, average="micro")
all_results[train_percent].append(result)
```

Node in graph may have multiple labels, so we conduct multilbel classification built from TopKRanker.

```
from sklearn.multiclass import OneVsRestClassifier

class TopKRanker(OneVsRestClassifier):
    def predict(self, X, top_k_list):
        assert X.shape[0] == len(top_k_list)
        probs = np.asarray(super(TopKRanker, self).predict_proba(X))
        all_labels = sp.lil_matrix(probs.shape)

        for i, k in enumerate(top_k_list):
            probs_ = probs[i, :]
            labels = self.classes_[probs_.argsort()[-k:]].tolist()
            for label in labels:
                all_labels[i, label] = 1
        return all_labels
```

Finally, we get the results of Micro-F1 score under different training ratio for different models on datasets.

```
return dict(
    (
        f"Micro-F1 {train_percent}",
        sum(all_results[train_percent]) / len(all_results[train_percent]),
    )
    for train_percent in sorted(all_results.keys())
)
```

The overall implementation of *UnsupervisedNodeClassification* is at (https://github.com/THUDM/cogdl/blob/master/cogdl/tasks/unsupervised_node_classification.py).

To run UnsupervisedNodeClassification, we can use following instruction:

```
python scripts/train.py --task unsupervised_node_classification --dataset ppi␣
↪wikipedia --model deepwalk prone -seed 0 1
```

Then We get experimental results like this:

Variant	Micro-F1 0.1	Micro-F1 0.3	Micro-F1 0.5	Micro-F1 0.7	Micro-F1 0.9
('ppi', 'deepwalk')	0.1547±0.0002	0.1846±0.0002	0.2033±0.0015	0.2161±0.0009	0.2243±0.0018
('ppi', 'prone')	0.1777±0.0016	0.2214±0.0020	0.2397±0.0015	0.2486±0.0022	0.2607±0.0096
('wikipedia', 'deepwalk')	0.4255±0.0027	0.4712±0.0005	0.4916±0.0011	0.5011±0.0017	0.5166±0.0043
('wikipedia', 'prone')	0.4834±0.0009	0.5320±0.0020	0.5504±0.0045	0.5586±0.0022	0.5686±0.0072

3.3 Supervised Graph Classification

In this section, we will introduce the implementation "Graph classification task".

Task Design

1. Set up "SupervisedGraphClassification" class, which has two specific parameters.
    - *degree-feature*: Use one-hot node degree as node feature, for datasets such as lmdb-binary and lmdb-multi, which don't have node features.
    - *gamma*: Multiplicative factor of learning rate decay.
    - *lr*: Learning rate.
2. Build dataset convert it to a list of *Data* defined in Cogdl. Specially, we reformat the data according to the input format of specific models. *generate_data* is implemented to convert dataset.

```
dataset = build_dataset(args)
self.data = self.generate_data(dataset, args)

def generate_data(self, dataset, args):
     if "ModelNet" in str(type(dataset).__name__):
         train_set, test_set = dataset.get_all()
         args.num_features = 3
         return {"train": train_set, "test": test_set}
    else:
        datalist = []
        if isinstance(dataset[0], Data):
            return dataset
        for idata in dataset:
            data = Data()
            for key in idata.keys:
                data[key] = idata[key]
                datalist.append(data)

        if args.degree_feature:
            datalist = node_degree_as_feature(datalist)
            args.num_features = datalist[0].num_features
        return datalist
```

3. Then we build model and can run *train* to train the model.

```
def train(self):
    for epoch in epoch_iter:
         self._train_step()
         val_acc, val_loss = self._test_step(split="valid")
         # ...
         return dict(Acc=test_acc)

def _train_step(self):
    self.model.train()
    loss_n = 0
    for batch in self.train_loader:
        batch = batch.to(self.device)
        self.optimizer.zero_grad()
        output, loss = self.model(batch)
        loss_n += loss.item()
        loss.backward()
        self.optimizer.step()

def _test_step(self, split):
    """split in ['train', 'test', 'valid']"""
    # ...
    return acc, loss
```

The overall implementation of GraphClassification is at (https://github.com/THUDM/cogdl/blob/master/cogdl/tasks/graph_classification.py).

Create a model

To create a model for task graph classification, the following functions have to be implemented.

1. *add_args(parser)*: add necessary hyper-parameters used in model.

```
@staticmethod
def add_args(parser):
     parser.add_argument("--hidden-size", type=int, default=128)
     parser.add_argument("--num-layers", type=int, default=2)
     parser.add_argument("--lr", type=float, default=0.001)
     # ...
```

2. *build_model_from_args(cls, args)*: this function is called in 'task' to build model.
3. *split_dataset(cls, dataset, args)*: split train/validation/test data and return correspondent dataloader according to requirement of model.

```
def split_dataset(cls, dataset, args):
    random.shuffle(dataset)
    train_size = int(len(dataset) * args.train_ratio)
    test_size = int(len(dataset) * args.test_ratio)
    bs = args.batch_size
    train_loader = DataLoader(dataset[:train_size], batch_size=bs)
    test_loader = DataLoader(dataset[-test_size:], batch_size=bs)
    if args.train_ratio + args.test_ratio < 1:
         valid_loader = DataLoader(dataset[train_size:-test_size], batch_size=bs)
    else:
         valid_loader = test_loader
    return train_loader, valid_loader, test_loader
```

4. *forward*: forward propagation, and the return should be (predication, loss) or (prediction, None), respectively for training and test. Input parameters of *forward* is class *Batch*, which

```
def forward(self, batch):
 h = batch.x
 layer_rep = [h]
 for i in range(self.num_layers-1):
     h = self.gin_layers[i](h, batch.edge_index)
     h = self.batch_norm[i](h)
     h = F.relu(h)
     layer_rep.append(h)

 final_score = 0
 for i in range(self.num_layers):
 pooled = scatter_add(layer_rep[i], batch.batch, dim=0)
 final_score += self.dropout(self.linear_prediction[i](pooled))
 final_score = F.softmax(final_score, dim=-1)
 if batch.y is not None:
     loss = self.loss(final_score, batch.y)
     return final_score, loss
 return final_score, None
```

Run

To run GraphClassification, we can use the following command:

```
python scripts/train.py --task graph_classification --dataset proteins --model gin␣
↪diffpool sortpool dgcnn --seed 0 1
```

Then We get experimental results like this:

Variants	Acc
('proteins', 'gin')	0.7286±0.0598
('proteins', 'diffpool')	0.7530±0.0589
('proteins', 'sortpool')	0.7411±0.0269
('proteins', 'dgcnn')	0.6677±0.0355
('proteins', 'patchy_san')	0.7550±0.0812

3.4 Unsupervised Graph Classification

In this section, we will introduce the implementation "Unsupervised graph classification task".

Task Design

1. Set up "UnsupervisedGraphClassification" class, which has two specific parameters.
    - *num-shuffle* : Shuffle times in classifier
    - *degree-feature*: Use one-hot node degree as node feature, for datasets such as lmdb-binary and lmdb-multi, which don't have node features.
    - *lr*: learning

```
@register_task("unsupervised_graph_classification")
class UnsupervisedGraphClassification(BaseTask):
    r"""Unsupervised graph classification"""
    @staticmethod
    def add_args(parser):
        """Add task-specific arguments to the parser."""
```

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```
        # fmt: off
        parser.add_argument("--num-shuffle", type=int, default=10)
        parser.add_argument("--degree-feature", dest="degree_feature", action="store_
↪true")
        parser.add_argument("--lr", type=float, default=0.001)
        # fmt: on
    def __init__(self, args):
        # ...
```

2. Build dataset and convert it to a list of *Data* defined in Cogdl.

```
dataset = build_dataset(args)
self.label = np.array([data.y for data in dataset])
self.data = [
     Data(x=data.x, y=data.y, edge_index=data.edge_index, edge_attr=data.edge_attr,
             pos=data.pos).apply(lambda x:x.to(self.device))
             for data in dataset
]
```

3. Then we build model and can run *train* to train the model and obtain graph representation. In this part, the training process of shallow models and deep models are implemented separately.

```
self.model = build_model(args)
self.model = self.model.to(self.device)

def train(self):
     if self.use_nn:
         # deep neural network models
              epoch_iter = tqdm(range(self.epoch))
         for epoch in epoch_iter:
             loss_n = 0
             for batch in self.data_loader:
                 batch = batch.to(self.device)
                 predict, loss = self.model(batch.x, batch.edge_index, batch.batch)
              self.optimizer.zero_grad()
              loss.backward()
              self.optimizer.step()
              loss_n += loss.item()
     # ...
     else:
        # shallow models
         prediction, loss = self.model(self.data)
         label = self.label
```

4. When graph representation is obtained, we evaluate the embedding with *SVM* via running *num_shuffle* times under different training ratio. You can also call *save_emb* to save the embedding.

```
return self._evaluate(prediction, label)
def _evaluate(self, embedding, labels):
    # ...
    for training_percent in training_percents:
         for shuf in shuffles:
             # ...
             clf = SVC()
             clf.fit(X_train, y_train)
             preds = clf.predict(X_test)
```

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```
            # ...
```

The overall implementation of UnsupervisedGraphClassification is at (https://github.com/THUDM/cogdl/blob/master/cogdl/tasks/unsupervised_graph_classification.py).

Create a model

To create a model for task unsupervised graph classification, the following functions have to be implemented.

1. *add_args(parser)*: add necessary hyper-parameters used in model.

```
@staticmethod
def add_args(parser):
  parser.add_argument("--hidden-size", type=int, default=128)
  parser.add_argument("--nn", type=bool, default=False)
  parser.add_argument("--lr", type=float, default=0.001)
  # ...
```

2. *build_model_from_args(cls, args)*: this function is called in 'task' to build model.
3. *forward*: For shallow models, this function runs as training process of model and will be called only once; For deep neural network models, this function is actually the forward propagation process and will be called many times.

```
# shallow model
def forward(self, graphs):
     # ...
    self.model = Doc2Vec(
        self.doc_collections,
             ...
    )
    vectors = np.array([self.model["g_"+str(i)] for i in range(len(graphs))])
    return vectors, None
```

Run

To run UnsupervisedGraphClassification, we can use the following command:

```
python scripts/train.py --task unsupervised_graph_classification --dataset proteins --
↪model dgk graph2vec
```

Then we get experimental results like this:

Variant	Acc
('proteins', 'dgk')	0.7259±0.0118
('proteins', 'graph2vec')	0.7330±0.0043
('proteins', 'infograph')	0.7393±0.0070

CHAPTER

FOUR

LICENSE

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CHAPTER

FIVE

CITING

- [Perozzi et al. (2014): Deepwalk: Online learning of social representations](http://arxiv.org/abs/1403.6652)
- [Tang et al. (2015): Line: Large-scale informa- tion network embedding](http://arxiv.org/abs/1503.03578)
- [Grover and Leskovec. (2016): node2vec: Scalable feature learning for networks](http://dl.acm.org/citation.cfm?doid=2939672.2939754)- [Cao et al. (2015):Grarep: Learning graph representations with global structural information](http://dl.acm.org/citation.cfm?doid=2806416.2806512)
- [Ou et al. (2016): Asymmetric transitivity preserving graph em- bedding](http://dl.acm.org/citation.cfm?doid=2939672.2939751)
- [Qiu et al. (2017): Network Embedding as Matrix Factorization: Unifying DeepWalk, LINE, PTE, and node2vec](http://arxiv.org/abs/1710.02971)
- [Qiu et al. (2019): NetSMF: Large-Scale Network Embedding as Sparse Matrix Factorization](http://arxiv.org/abs/1710.02971)
- [Zhang et al. (2019): Spectral Network Embedding: A Fast and Scalable Method via Sparsity](http://arxiv.org/abs/1806.02623)
- [Kipf and Welling (2016): Semi-Supervised Classification with Graph Convolutional Networks](https://arxiv.org/abs/1609.02907)
- [Hamilton et al. (2017): Inductive Representation Learning on Large Graphs](https://arxiv.org/abs/1706.02216)
- [Veličković et al. (2017): Graph Attention Networks](https://arxiv.org/abs/1710.10903)
- [Ding et al. (2018): Semi-supervised Learning on Graphs with Generative Adversarial Nets](https://arxiv.org/abs/1809.00130)
- [Han et al. (2019): GroupRep: Unsupervised Structural Representation Learning for Groups in Networks](https://www.overleaf.com/read/nqxjtkmmgmff)
- [Zhang et al. (2019): Revisiting Graph Convolutional Networks: Neighborhood Aggregation and Network Sampling](https://www.overleaf.com/read/xzykmvhxjmxy)
- [Zhang et al. (2019): Co-training Graph Convolutional Networks with Network Redundancy](https://www.overleaf.com/read/fbhqqgzqgmyn)
- [Qiu et al. (2019): NetSMF: Large-Scale Network Embedding as Sparse Matrix Factorization](http://keg.cs.tsinghua.edu.cn/jietang/publications/www19-Qiu-et-al-NetSMF-Large-Scale-Network-Embedding.pdf)
- [Zhang et al. (2019): ProNE: Fast and Scalable Network Representation Learning](https://www.overleaf.com/read/dhgpkmyfdhnj)
- [Cen et al. (2019): Representation Learning for Attributed Multiplex Heterogeneous Network](https://arxiv.org/abs/1905.01669)

CHAPTER

SIX

API REFERENCE

This page contains auto-generated API reference documentation[1].

6.1 cogdl

6.1.1 Subpackages

cogdl.data

Submodules

cogdl.data.batch

Module Contents

Classes

Batch	A plain old python object modeling a batch of graphs as one big

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

Bases: *cogdl.data.Data*

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.

static from_data_list(*data_list*, *follow_batch=[]*)

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

cumsum(*self*, *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

[1] Created with sphinx-autoapi

process is corrupted for a specific data attribute.

to_data_list(*self*)
Reconstructs the list of `torch_geometric.data.Data` objects from the batch object. The batch object must have been created via *`from_data_list()`* in order to be able reconstruct the initial objects.

property num_graphs(*self*)
Returns the number of graphs in the batch.

cogdl.data.data

Module Contents

Classes

Data	A plain old python object modeling a single graph with various

class cogdl.data.data.**Data**(*x=None*, *edge_index=None*, *edge_attr=None*, *y=None*, *pos=None*)
Bases: `object`

A plain old python object modeling a single graph with various (optional) attributes:

Args:

**x (Tensor, optional): Node feature matrix with shape :obj:`[num_nodes,** num_node_features]`. (default: `None`)

edge_index (LongTensor, optional): Graph connectivity in COO format with shape `[2, num_edges]`. (default: `None`)

edge_attr (Tensor, optional): Edge feature matrix with shape `[num_edges, num_edge_features]`. (default: `None`)

y (Tensor, optional): Graph or node targets with arbitrary shape. (default: `None`)

pos (Tensor, optional): Node position matrix with shape `[num_nodes, num_dimensions]`. (default: `None`)

The data object is not restricted to these attributes and can be extented by any other additional data.

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

__getitem__(*self*, *key*)
Gets the data of the attribute `key`.

__setitem__(*self*, *key*, *value*)
Sets the attribute `key` to `value`.

property keys(*self*)
Returns all names of graph attributes.

__len__(*self*)
Returns the number of all present attributes.

__contains__(*self*, *key*)
Returns `True`, if the attribute `key` is present in the data.

__iter__(*self*)
Iterates over all present attributes in the data, yielding their attribute names and content.

__call__(*self*, **keys*)
Iterates over all attributes `*keys` in the data, yielding their attribute names and content. If `*keys` is not given this method will iterative over all present attributes.

cat_dim(*self*, *key*, *value*)
Returns the dimension in which the attribute `key` with content `value` gets concatenated when creating batches.

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.

__inc__(*self*, *key*, *value*)
"Returns the incremental count to cumulatively increase the value of the next attribute of `key` when creating batches.

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.

---

property num_edges(*self*)
Returns the number of edges in the graph.

property num_features(*self*)
Returns the number of features per node in the graph.

property num_nodes(*self*)

is_coalesced(*self*)
Returns `True`, if edge indices are ordered and do not contain duplicate entries.

apply(*self*, *func*, **keys*)
Applies the function `func` to all attributes `*keys`. If `*keys` is not given, `func` is applied to all present attributes.

contiguous(*self*, **keys*)
Ensures a contiguous memory layout for all attributes `*keys`. If `*keys` is not given, all present attributes are ensured to have a contiguous memory layout.

to(*self*, *device*, **keys*)
Performs tensor dtype and/or device conversion to all attributes `*keys`. If `*keys` is not given, the conversion is applied to all present attributes.

cuda(*self*, **keys*)

clone(*self*)

__repr__(*self*)
Return repr(self).

cogdl.data.dataloader

Module Contents

Classes

DataLoader	Data loader which merges data objects from a
DataListLoader	Data loader which merges data objects from a
DenseDataLoader	Data loader which merges data objects from a

class cogdl.data.dataloader.**DataLoader**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)

Bases: torch.utils.data.DataLoader

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

Args: 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)

class cogdl.data.dataloader.**DataListLoader**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)

Bases: torch.utils.data.DataLoader

Data loader which merges data objects from a *cogdl.data.dataset* to a python list.

Note: This data loader should be used for multi-gpu support via cogdl.nn.DataParallel.

Args: 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)

class cogdl.data.dataloader.**DenseDataLoader**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)

Bases: torch.utils.data.DataLoader

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

Note: To make use of this data loader, all graphs in the dataset needs to have the same shape for each its attributes. Therefore, this data loader should only be used when working with *dense* adjacency matrices.

Args: 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)

cogdl.data.dataset

Module Contents

Classes

Dataset	Dataset base class for creating graph datasets.

Functions

to_list(x)	
files_exist(files)	

cogdl.data.dataset.**to_list**(*x*)

cogdl.data.dataset.**files_exist**(*files*)

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

Bases: torch.utils.data.Dataset

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

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

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

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

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

abstract __len__(*self*)
The number of examples in the dataset.

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

property num_features(*self*)
Returns the number of features per node in the graph.

property raw_paths(*self*)
The filepaths to find in order to skip the download.

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

_download(*self*)

_process(*self*)

__getitem__(*self*, *idx*)
Gets the data object at index `idx` and transforms it (in case a `self.transform` is given).

__repr__(*self*)

cogdl.data.download

Module Contents

Functions

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

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

Args: url (string): The url. folder (string): The folder. log (bool, optional): If `False`, will not print anything to the

console. (default: `True`)

cogdl.data.extract

Module Contents

Functions

maybe_log(path, log=True)	
extract_tar(path, folder, mode='r:gz', log=True)	Extracts a tar archive to a specific folder.
extract_zip(path, folder, log=True)	Extracts a zip archive to a specific folder.
extract_bz2(path, folder, log=True)	
extract_gz(path, folder, log=True)	

cogdl.data.extract.**maybe_log**(*path*, *log=True*)

cogdl.data.extract.**extract_tar**(*path*, *folder*, *mode='r:gz'*, *log=True*)
Extracts a tar archive to a specific folder.

Args: path (string): The path to the tar archive. folder (string): The folder. mode (string, optional): The compression mode. (default: `"r:gz"`) log (bool, optional): If `False`, will not print anything to the

console. (default: `True`)

cogdl.data.extract.**extract_zip**(*path*, *folder*, *log=True*)
Extracts a zip archive to a specific folder.

Args: path (string): The path to the tar archive. folder (string): The folder. log (bool, optional): If `False`, will not print anything to the

console. (default: `True`)

cogdl.data.extract.**extract_bz2**(*path*, *folder*, *log=True*)

cogdl.data.extract.**extract_gz**(*path*, *folder*, *log=True*)

cogdl.data.makedirs

Module Contents

Functions

makedirs(path)

cogdl.data.makedirs.**makedirs**(*path*)

cogdl.data.sampler

Module Contents

Classes

Sampler
SAINTSampler
NodeSampler
EdgeSampler
RWSampler
MRWSampler
LayerSampler

class cogdl.data.sampler.**Sampler**(*data*, *args_params*)

sample(*self*)

class cogdl.data.sampler.**SAINTSampler**(*data*, *args_params*)
Bases: *cogdl.data.sampler.Sampler*

estimate(*self*)

gen_subgraph(*self*)

sample(*self*)

extract_subgraph(*self*, *edge_idx*, *directed=True*)

get_subgraph(*self*, *phase*, *require_norm=True*)
Generate one minibatch for model. In the 'train' mode, one minibatch corresponds to one subgraph of the training graph. In the 'valid' or 'test' mode, one batch corresponds to the full graph (i.e., full-batch rather than minibatch evaluation for validation / test sets).

Inputs: mode str, can be 'train', 'valid', 'test' require_norm boolean

Outputs: data Data object, modeling the sampled subgraph data.norm_aggr aggregation normalization data.norm_loss normalization normalization

class cogdl.data.sampler.**NodeSampler**(*data*, *args_params*)
Bases: *cogdl.data.sampler.SAINTSampler*

sample(*self*)

class cogdl.data.sampler.**EdgeSampler**(*data*, *args_params*)
Bases: *cogdl.data.sampler.SAINTSampler*

sample(*self*)

class cogdl.data.sampler.**RWSampler**(*data*, *args_params*)
Bases: *cogdl.data.sampler.SAINTSampler*

sample(*self*)

class cogdl.data.sampler.**MRWSampler**(*data*, *args_params*)
Bases: *cogdl.data.sampler.SAINTSampler*

sample(*self*)

class cogdl.data.sampler.**LayerSampler**(*data*, *model*, *params_args*)
Bases: *cogdl.data.sampler.Sampler*

get_batches(*self*, *train_nodes*, *train_labels*, *batch_size=64*, *shuffle=True*)

Package Contents

Classes

Data	A plain old python object modeling a single graph with various
Batch	A plain old python object modeling a batch of graphs as one big
Dataset	Dataset base class for creating graph datasets.

continues on next page

Table 10 – continued from previous page

DataLoader	Data loader which merges data objects from a
DataListLoader	Data loader which merges data objects from a
DenseDataLoader	Data loader which merges data objects from a

Functions

download_url(url, folder, name=None, log=True)	Downloads the content of an URL to a specific folder.
extract_tar(path, folder, mode='r:gz', log=True)	Extracts a tar archive to a specific folder.
extract_zip(path, folder, log=True)	Extracts a zip archive to a specific folder.
extract_bz2(path, folder, log=True)	
extract_gz(path, folder, log=True)	

class cogdl.data.**Data**(*x=None*, *edge_index=None*, *edge_attr=None*, *y=None*, *pos=None*)

Bases: object

A plain old python object modeling a single graph with various (optional) attributes:

Args:

**x (Tensor, optional): Node feature matrix with shape :obj:`[num_nodes,** num_node_features]`. (default: None)

edge_index (LongTensor, optional): Graph connectivity in COO format with shape [2, num_edges]. (default: None)

edge_attr (Tensor, optional): Edge feature matrix with shape [num_edges, num_edge_features]. (default: None)

y (Tensor, optional): Graph or node targets with arbitrary shape. (default: None)

pos (Tensor, optional): Node position matrix with shape [num_nodes, num_dimensions]. (default: None)

The data object is not restricted to these attributes and can be extented by any other additional data.

static from_dict(*dictionary*)

Creates a data object from a python dictionary.

__getitem__(*self*, *key*)

Gets the data of the attribute key.

__setitem__(*self*, *key*, *value*)

Sets the attribute key to value.

property keys(*self*)

Returns all names of graph attributes.

__len__(*self*)

Returns the number of all present attributes.

__contains__(*self*, *key*)

Returns True, if the attribute key is present in the data.

__iter__(*self*)

Iterates over all present attributes in the data, yielding their attribute names and content.

__call__(*self*, **keys*)
Iterates over all attributes `*keys` in the data, yielding their attribute names and content. If `*keys` is not given this method will iterative over all present attributes.

cat_dim(*self*, *key*, *value*)
Returns the dimension in which the attribute `key` with content `value` gets concatenated when creating batches.

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.

__inc__(*self*, *key*, *value*)
"Returns the incremental count to cumulatively increase the value of the next attribute of `key` when creating batches.

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.

---

property num_edges(*self*)
Returns the number of edges in the graph.

property num_features(*self*)
Returns the number of features per node in the graph.

property num_nodes(*self*)

is_coalesced(*self*)
Returns `True`, if edge indices are ordered and do not contain duplicate entries.

apply(*self*, *func*, **keys*)
Applies the function `func` to all attributes `*keys`. If `*keys` is not given, `func` is applied to all present attributes.

contiguous(*self*, **keys*)
Ensures a contiguous memory layout for all attributes `*keys`. If `*keys` is not given, all present attributes are ensured to have a contiguous memory layout.

to(*self*, *device*, **keys*)
Performs tensor dtype and/or device conversion to all attributes `*keys`. If `*keys` is not given, the conversion is applied to all present attributes.

cuda(*self*, **keys*)

clone(*self*)

__repr__(*self*)
Return repr(self).

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

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.

static from_data_list(*data_list*, *follow_batch=[]*)
Constructs a batch object from a python list holding `torch_geometric.data.Data` objects. The

assignment vector *batch* is created on the fly. Additionally, creates assignment batch vectors for each key in follow_batch.

cumsum(*self*, *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.

---

to_data_list(*self*)
Reconstructs the list of torch_geometric.data.Data objects from the batch object. The batch object must have been created via *from_data_list()* in order to be able reconstruct the initial objects.

property num_graphs(*self*)
Returns the number of graphs in the batch.

class cogdl.data.**Dataset**(*root*, *transform=None*, *pre_transform=None*, *pre_filter=None*)
Bases: torch.utils.data.Dataset

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

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

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

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

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

abstract __len__(*self*)
The number of examples in the dataset.

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

property num_features(*self*)
Returns the number of features per node in the graph.

property raw_paths(*self*)
The filepaths to find in order to skip the download.

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

_download(*self*)

_process(*self*)

__getitem__(*self*, *idx*)
Gets the data object at index `idx` and transforms it (in case a `self.transform` is given).

__repr__(*self*)

class cogdl.data.**DataLoader**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)
Bases: `torch.utils.data.DataLoader`

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

Args: 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`)

class cogdl.data.**DataListLoader**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)
Bases: `torch.utils.data.DataLoader`

Data loader which merges data objects from a *cogdl.data.dataset* to a python list.

Note: This data loader should be used for multi-gpu support via `cogdl.nn.DataParallel`.

Args: 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`)

class cogdl.data.**DenseDataLoader**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)
Bases: `torch.utils.data.DataLoader`

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

Note: To make use of this data loader, all graphs in the dataset needs to have the same shape for each its attributes. Therefore, this data loader should only be used when working with *dense* adjacency matrices.

Args: 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`)

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

Args: url (string): The url. folder (string): The folder. log (bool, optional): If `False`, will not print anything to the

console. (default: `True`)

cogdl.data.**extract_tar**(*path*, *folder*, *mode='r:gz'*, *log=True*)
Extracts a tar archive to a specific folder.

Args: path (string): The path to the tar archive. folder (string): The folder. mode (string, optional): The compression mode. (default: `"r:gz"`) log (bool, optional): If `False`, will not print anything to the

console. (default: `True`)

cogdl.data.**extract_zip**(*path*, *folder*, *log=True*)
Extracts a zip archive to a specific folder.

Args: path (string): The path to the tar archive. folder (string): The folder. log (bool, optional): If `False`, will not print anything to the

console. (default: `True`)

cogdl.data.**extract_bz2**(*path*, *folder*, *log=True*)

cogdl.data.**extract_gz**(*path*, *folder*, *log=True*)

cogdl.datasets

Submodules

cogdl.datasets.dgl_data

Module Contents

Classes

MUTAGDataset
CollabDataset
ImdbBinaryDataset
ImdbMultiDataset
ProtainsDataset

class cogdl.datasets.dgl_data.**MUTAGDataset**
Bases: dgl.data.tu.TUDataset

class cogdl.datasets.dgl_data.**CollabDataset**
Bases: dgl.data.tu.TUDataset

class cogdl.datasets.dgl_data.**ImdbBinaryDataset**
Bases: dgl.data.tu.TUDataset

class cogdl.datasets.dgl_data.**ImdbMultiDataset**
Bases: dgl.data.tu.TUDataset

class cogdl.datasets.dgl_data.**ProtainsDataset**
Bases: dgl.data.tu.TUDataset

cogdl.datasets.gatne

Module Contents

Classes

GatneDataset	The network datasets “Amazon”, “Twitter” and “YouTube” from the
AmazonDataset	The network datasets “Amazon”, “Twitter” and “YouTube” from the
TwitterDataset	The network datasets “Amazon”, “Twitter” and “YouTube” from the
YouTubeDataset	The network datasets “Amazon”, “Twitter” and “YouTube” from the

Functions

read_gatne_data(folder)	

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

class cogdl.datasets.gatne.**GatneDataset**(*root*, *name*)
Bases: *cogdl.data.Dataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"Amazon"`,

`"Twitter"`, `"YouTube"`).

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

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

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

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

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

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

__repr__(*self*)

class cogdl.datasets.gatne.**AmazonDataset**
Bases: *cogdl.datasets.gatne.GatneDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset ("Amazon",

"Twitter", "YouTube").

class cogdl.datasets.gatne.**TwitterDataset**
Bases: *cogdl.datasets.gatne.GatneDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset ("Amazon",

"Twitter", "YouTube").

class cogdl.datasets.gatne.**YouTubeDataset**
Bases: *cogdl.datasets.gatne.GatneDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset ("Amazon",

"Twitter", "YouTube").

cogdl.datasets.gcc_data

Module Contents

Classes

Edgelist	Dataset base class for creating graph datasets.
USAAirportDataset	Dataset base class for creating graph datasets.

class cogdl.datasets.gcc_data.**Edgelist**(*root*, *name*)
Bases: *cogdl.data.Dataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

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

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

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

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

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

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

class cogdl.datasets.gcc_data.**USAAirportDataset**
Bases: *cogdl.datasets.gcc_data.Edgelist*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

cogdl.datasets.gtn_data

Module Contents

Classes

GTNDataset	The network datasets "ACM", "DBLP" and "IMDB" from the
ACM_GTNDataset	The network datasets "ACM", "DBLP" and "IMDB" from the
DBLP_GTNDataset	The network datasets "ACM", "DBLP" and "IMDB" from the
IMDB_GTNDataset	The network datasets "ACM", "DBLP" and "IMDB" from the

Functions

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

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

class cogdl.datasets.gtn_data.**GTNDataset**(*root*, *name*)
Bases: *cogdl.data.Dataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset ("gtn-acm",

"gtn-dblp", "gtn-imdb").

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

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

read_gtn_data(*self*, *folder*)

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

apply_to_device(*self*, *device*)

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

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

__repr__(*self*)

class cogdl.datasets.gtn_data.**ACM_GTNDataset**
Bases: *cogdl.datasets.gtn_data.GTNDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset ("gtn-acm",

"gtn-dblp", "gtn-imdb").

class cogdl.datasets.gtn_data.**DBLP_GTNDataset**
Bases: *cogdl.datasets.gtn_data.GTNDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset ("gtn-acm",

"gtn-dblp", "gtn-imdb").

class cogdl.datasets.gtn_data.**IMDB_GTNDataset**
Bases: *cogdl.datasets.gtn_data.GTNDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"gtn-acm"`,

`"gtn-dblp"`, `"gtn-imdb"`).

cogdl.datasets.han_data

Module Contents

Classes

HANDataset	The network datasets "ACM", "DBLP" and "IMDB" from the
ACM_HANDataset	The network datasets "ACM", "DBLP" and "IMDB" from the
DBLP_HANDataset	The network datasets "ACM", "DBLP" and "IMDB" from the
IMDB_HANDataset	The network datasets "ACM", "DBLP" and "IMDB" from the

Functions

untar(path, fname, deleteTar=True)	Unpacks the given archive file to the same directory, then (by default)
sample_mask(idx, l)	Create mask.

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

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

class cogdl.datasets.han_data.**HANDataset**(*root*, *name*)
Bases: *cogdl.data.Dataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"han-acm"`,

`"han-dblp"`, `"han-imdb"`).

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

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

read_gtn_data(*self*, *folder*)

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

apply_to_device(*self*, *device*)

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

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

__repr__(*self*)

class cogdl.datasets.han_data.**ACM_HANDataset**
Bases: *cogdl.datasets.han_data.HANDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"han-acm"`,

`"han-dblp"`, `"han-imdb"`).

class cogdl.datasets.han_data.**DBLP_HANDataset**
Bases: *cogdl.datasets.han_data.HANDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"han-acm"`,

`"han-dblp"`, `"han-imdb"`).

class cogdl.datasets.han_data.**IMDB_HANDataset**
Bases: *cogdl.datasets.han_data.HANDataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"han-acm"`,

`"han-dblp"`, `"han-imdb"`).

cogdl.datasets.kg_data

Module Contents

Classes

BidirectionalOneShotIterator	
TestDataset	
TrainDataset	
KnowledgeGraphDataset	Dataset base class for creating graph datasets.
FB13Datset	Dataset base class for creating graph datasets.
FB15kDatset	Dataset base class for creating graph datasets.
FB15k237Datset	Dataset base class for creating graph datasets.
WN18Datset	Dataset base class for creating graph datasets.
WN18RRDataset	Dataset base class for creating graph datasets.
FB13SDatset	Dataset base class for creating graph datasets.

Functions

read_triplet_data(folder)

class cogdl.datasets.kg_data.**BidirectionalOneShotIterator**(*dataloader_head*, *dataloader_tail*)

Bases: object

__next__(*self*)

static one_shot_iterator(*dataloader*)
Transform a PyTorch Dataloader into python iterator

class cogdl.datasets.kg_data.**TestDataset**(*triples*, *all_true_triples*, *nentity*, *nrelation*, *mode*)

Bases: torch.utils.data.Dataset

__len__(*self*)

__getitem__(*self*, *idx*)

static collate_fn(*data*)

class cogdl.datasets.kg_data.**TrainDataset**(*triples*, *nentity*, *nrelation*, *negative_sample_size*, *mode*)

Bases: torch.utils.data.Dataset

__len__(*self*)

__getitem__(*self*, *idx*)

static collate_fn(*data*)

static count_frequency(*triples*, *start=4*)
Get frequency of a partial triple like (head, relation) or (relation, tail) The frequency will be used for subsampling like word2vec

static get_true_head_and_tail(*triples*)
Build a dictionary of true triples that will be used to filter these true triples for negative sampling

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

class cogdl.datasets.kg_data.**KnowledgeGraphDataset**(*root*, *name*)

Bases: *cogdl.data.Dataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

url = https://raw.githubusercontent.com/thunlp/OpenKE/OpenKE-PyTorch/benchmarks

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

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

property train_start_idx(*self*)

property valid_start_idx(*self*)

property test_start_idx(*self*)

property num_entities(*self*)

property num_relations(*self*)

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

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

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

class cogdl.datasets.kg_data.**FB13Datset**
Bases: *cogdl.datasets.kg_data.KnowledgeGraphDataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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`)

class cogdl.datasets.kg_data.**FB15kDatset**
Bases: *cogdl.datasets.kg_data.KnowledgeGraphDataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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`)

class cogdl.datasets.kg_data.**FB15k237Datset**
Bases: *cogdl.datasets.kg_data.KnowledgeGraphDataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

class cogdl.datasets.kg_data.**WN18Datset**
Bases: *cogdl.datasets.kg_data.KnowledgeGraphDataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

class cogdl.datasets.kg_data.**WN18RRDataset**
Bases: *cogdl.datasets.kg_data.KnowledgeGraphDataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

class cogdl.datasets.kg_data.**FB13SDatset**
Bases: *cogdl.datasets.kg_data.KnowledgeGraphDataset*

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

url = https://raw.githubusercontent.com/cenyk1230/test-data/main

cogdl.datasets.matlab_matrix

Module Contents

Classes

MatlabMatrix	networks from the http://leitang.net/code/social-dimension/data/ or http://snap.stanford.edu/node2vec/
BlogcatalogDataset	networks from the http://leitang.net/code/social-dimension/data/ or http://snap.stanford.edu/node2vec/
FlickrDataset	networks from the http://leitang.net/code/social-dimension/data/ or http://snap.stanford.edu/node2vec/
WikipediaDataset	networks from the http://leitang.net/code/social-dimension/data/ or http://snap.stanford.edu/node2vec/
PPIDataset	networks from the http://leitang.net/code/social-dimension/data/ or http://snap.stanford.edu/node2vec/

class cogdl.datasets.matlab_matrix.**MatlabMatrix**(*root*, *name*, *url*)

Bases: *cogdl.data.Dataset*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"Blogcatalog"`).

property raw_file_names(*self*)

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

property processed_file_names(*self*)

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

download(*self*)

Downloads the dataset to the `self.raw_dir` folder.

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

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

class cogdl.datasets.matlab_matrix.**BlogcatalogDataset**
Bases: *cogdl.datasets.matlab_matrix.MatlabMatrix*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"Blogcatalog"`).

class cogdl.datasets.matlab_matrix.**FlickrDataset**
Bases: *cogdl.datasets.matlab_matrix.MatlabMatrix*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"Blogcatalog"`).

class cogdl.datasets.matlab_matrix.**WikipediaDataset**
Bases: *cogdl.datasets.matlab_matrix.MatlabMatrix*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"Blogcatalog"`).

class cogdl.datasets.matlab_matrix.**PPIDataset**
Bases: *cogdl.datasets.matlab_matrix.MatlabMatrix*

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

Args: root (string): Root directory where the dataset should be saved. name (string): The name of the dataset (`"Blogcatalog"`).

cogdl.datasets.pyg

Module Contents

Classes

CoraDataset
CiteSeerDataset
PubMedDataset
RedditDataset
MUTAGDataset

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Table 23 – continued from previous page

ImdbBinaryDataset
ImdbMultiDataset
CollabDataset
ProtainsDataset
RedditBinary
RedditMulti5K
RedditMulti12K
PTCMRDataset
NCT1Dataset
NCT109Dataset
ENZYMES
QM9Dataset

Functions

normalize_feature(data)

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

class cogdl.datasets.pyg.**CoraDataset**
Bases: torch_geometric.datasets.Planetoid

class cogdl.datasets.pyg.**CiteSeerDataset**
Bases: torch_geometric.datasets.Planetoid

class cogdl.datasets.pyg.**PubMedDataset**
Bases: torch_geometric.datasets.Planetoid

class cogdl.datasets.pyg.**RedditDataset**
Bases: torch_geometric.datasets.Reddit

class cogdl.datasets.pyg.**MUTAGDataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**ImdbBinaryDataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**ImdbMultiDataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**CollabDataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**ProtainsDataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**RedditBinary**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**RedditMulti5K**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**RedditMulti12K**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**PTCMRDataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**NCT1Dataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**NCT109Dataset**
Bases: torch_geometric.datasets.TUDataset

class cogdl.datasets.pyg.**ENZYMES**
Bases: torch_geometric.datasets.TUDataset

__getitem__(*self*, *idx*)

class cogdl.datasets.pyg.**QM9Dataset**
Bases: torch_geometric.datasets.QM9

cogdl.datasets.pyg_ogb

Module Contents

Classes

OGBNDataset
OGBArxivDataset
OGBProductsDataset
OGBProductsDataset
OGBProductsDataset
OGBPapers100MDataset
OGBGDataset
OGBMolbaceDataset

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Table 25 – continued from previous page

OGBMolhivDataset
OGBMolpcbaDataset
OGBPpaDataset
OGBCodeDataset

class cogdl.datasets.pyg_ogb.**OGBNDataset**(*root*, *name*)
Bases: ogb.nodeproppred.PygNodePropPredDataset

get(*self*, *idx*)

class cogdl.datasets.pyg_ogb.**OGBArxivDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBNDataset*

class cogdl.datasets.pyg_ogb.**OGBProductsDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBNDataset*

class cogdl.datasets.pyg_ogb.**OGBProductsDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBNDataset*

class cogdl.datasets.pyg_ogb.**OGBProductsDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBNDataset*

class cogdl.datasets.pyg_ogb.**OGBPapers100MDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBNDataset*

class cogdl.datasets.pyg_ogb.**OGBGDataset**(*root*, *name*)
Bases: ogb.graphproppred.PygGraphPropPredDataset

get_loader(*self*, *args*)

get(*self*, *idx*)

class cogdl.datasets.pyg_ogb.**OGBMolbaceDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBGDataset*

class cogdl.datasets.pyg_ogb.**OGBMolhivDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBGDataset*

class cogdl.datasets.pyg_ogb.**OGBMolpcbaDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBGDataset*

class cogdl.datasets.pyg_ogb.**OGBPpaDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBGDataset*

class cogdl.datasets.pyg_ogb.**OGBCodeDataset**
Bases: *cogdl.datasets.pyg_ogb.OGBGDataset*

cogdl.datasets.pyg_strategies_data

This file is borrowed from https://github.com/snap-stanford/pretrain-gnns/

Module Contents

Classes

NegativeEdge	Borrowed from https://github.com/snap-stanford/pretrain-gnns/
MaskEdge	Borrowed from https://github.com/snap-stanford/pretrain-gnns/
MaskAtom	Borrowed from https://github.com/snap-stanford/pretrain-gnns/
ExtractSubstructureContextPair	
ChemExtractSubstructureContextPair	
BatchFinetune	
BatchMasking	
BatchAE	
BatchSubstructContext	
DataLoaderFinetune	
DataLoaderMasking	
DataLoaderAE	
DataLoaderSubstructContext	
TestBioDataset	
TestChemDataset	
BioDataset	
MoleculeDataset	
BACEDataset	
BBBPDataset	

Functions

nx_to_graph_data_obj(g, center_id, allowable_features_downstream=None, allowable_features_pretrain=None, node_id_to_go_labels=None)	
graph_data_obj_to_nx(data)	
graph_data_obj_to_nx_simple(data)	Converts graph Data object required by the pytorch geometric package to
nx_to_graph_data_obj_simple(G)	Converts nx graph to pytorch geometric Data object. Assume node indices
reset_idxes(G)	Resets node indices such that they are numbered from 0 to num_nodes - 1

cogdl.datasets.pyg_strategies_data.**nx_to_graph_data_obj**(*g*, *center_id*, *allowable_features_downstream=None*, *allowable_features_pretrain=None*, *node_id_to_go_labels=None*)

cogdl.datasets.pyg_strategies_data.**graph_data_obj_to_nx**(*data*)

cogdl.datasets.pyg_strategies_data.**graph_data_obj_to_nx_simple**(*data*)
Converts graph Data object required by the pytorch geometric package to network x data object. NB: Uses simplified atom and bond features, and represent as indices. NB: possible issues with recapitulating relative stereochemistry since the edges in the nx object are unordered. :param data: pytorch geometric Data object :return: network x object

cogdl.datasets.pyg_strategies_data.**nx_to_graph_data_obj_simple**(*G*)
Converts nx graph to pytorch geometric Data object. Assume node indices are numbered from 0 to num_nodes - 1. NB: Uses simplified atom and bond features, and represent as indices. NB: possible issues with recapitulating relative stereochemistry since the edges in the nx object are unordered. :param G: nx graph obj :return: pytorch geometric Data object

class cogdl.datasets.pyg_strategies_data.**NegativeEdge**
Borrowed from https://github.com/snap-stanford/pretrain-gnns/

__call__(*self*, *data*)

class cogdl.datasets.pyg_strategies_data.**MaskEdge**(*mask_rate*)
Borrowed from https://github.com/snap-stanford/pretrain-gnns/

__call__(*self*, *data*, *masked_edge_indices=None*)

class cogdl.datasets.pyg_strategies_data.**MaskAtom**(*num_atom_type*, *num_edge_type*, *mask_rate*, *mask_edge=True*)
Borrowed from https://github.com/snap-stanford/pretrain-gnns/

__call__(*self*, *data*, *masked_atom_indices=None*)

Parameters **data** – pytorch geometric data object. Assume that the edge

ordering is the default pytorch geometric ordering, where the two directions of a single edge occur in pairs. Eg. data.edge_index = tensor([[0, 1, 1, 2, 2, 3],

[1, 0, 2, 1, 3, 2]])

Parameters **masked_atom_indices** – If None, then randomly samples num_atoms

- mask rate number of atom indices

Otherwise a list of atom idx that sets the atoms to be masked (for debugging only) :return: None, Creates new attributes in original data object: data.mask_node_idx data.mask_node_label data.mask_edge_idx data.mask_edge_label

__repr__(*self*)
Return repr(self).

cogdl.datasets.pyg_strategies_data.**reset_idxes**(*G*)
Resets node indices such that they are numbered from 0 to num_nodes - 1 :param G: :return: copy of G with relabelled node indices, mapping

class cogdl.datasets.pyg_strategies_data.**ExtractSubstructureContextPair**(*l1*, *center=True*)

__call__(*self*, *data*, *root_idx=None*)

__repr__(*self*)
Return repr(self).

class cogdl.datasets.pyg_strategies_data.**ChemExtractSubstructureContextPair**(*k*, *l1*, *l2*)

__call__(*self*, *data*, *root_idx=None*)

Parameters

- **data** – pytorch geometric data object
- **root_idx** – If None, then randomly samples an atom idx.

Otherwise sets atom idx of root (for debugging only) :return: None. Creates new attributes in original data object: data.center_substruct_idx data.x_substruct data.edge_attr_substruct data.edge_index_substruct data.x_context data.edge_attr_context data.edge_index_context data.overlap_context_substruct_idx

__repr__(*self*)
Return repr(self).

class cogdl.datasets.pyg_strategies_data.**BatchFinetune**(*batch=None*, ***kwargs*)
Bases: torch_geometric.data.Data

static from_data_list(*data_list*)
Constructs a batch object from a python list holding torch_geometric.data.Data objects. The assignment vector batch is created on the fly.

property num_graphs(*self*)
Returns the number of graphs in the batch.

class cogdl.datasets.pyg_strategies_data.**BatchMasking**(*batch=None*, ***kwargs*)
Bases: torch_geometric.data.Data

static from_data_list(*data_list*)
Constructs a batch object from a python list holding torch_geometric.data.Data objects. The assignment vector batch is created on the fly.

cumsum(*self*, *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.
```

property num_graphs(*self*)
Returns the number of graphs in the batch.

class cogdl.datasets.pyg_strategies_data.**BatchAE**(*batch=None*, ***kwargs*)
Bases: torch_geometric.data.Data

static from_data_list(*data_list*)
Constructs a batch object from a python list holding torch_geometric.data.Data objects. The assignment vector batch is created on the fly.

property num_graphs(*self*)
Returns the number of graphs in the batch.

cat_dim(*self*, *key*)

class cogdl.datasets.pyg_strategies_data.**BatchSubstructContext**(*batch=None*, ***kwargs*)
Bases: torch_geometric.data.Data

static from_data_list(*data_list*)
Constructs a batch object from a python list holding torch_geometric.data.Data objects. The assignment vector batch is created on the fly.

cat_dim(*self*, *key*)

cumsum(*self*, *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.
```

property num_graphs(*self*)
Returns the number of graphs in the batch.

class cogdl.datasets.pyg_strategies_data.**DataLoaderFinetune**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)
Bases: torch.utils.data.DataLoader

class cogdl.datasets.pyg_strategies_data.**DataLoaderMasking**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)
Bases: torch.utils.data.DataLoader

class cogdl.datasets.pyg_strategies_data.**DataLoaderAE**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)
Bases: torch.utils.data.DataLoader

class cogdl.datasets.pyg_strategies_data.**DataLoaderSubstructContext**(*dataset*, *batch_size=1*, *shuffle=True*, ***kwargs*)
Bases: torch.utils.data.DataLoader

class cogdl.datasets.pyg_strategies_data.**TestBioDataset**(*data_type='unsupervised'*, *root=None*, *transform=None*, *pre_transform=None*, *pre_filter=None*)

Bases: torch_geometric.data.InMemoryDataset

class cogdl.datasets.pyg_strategies_data.**TestChemDataset**(*data_type='unsupervised'*, *root=None*, *transform=None*, *pre_transform=None*, *pre_filter=None*)

Bases: torch_geometric.data.InMemoryDataset

get(*self*, *idx*)

class cogdl.datasets.pyg_strategies_data.**BioDataset**(*data_type='unsupervised'*, *empty=False*, *transform=None*, *pre_transform=None*, *pre_filter=None*)

Bases: torch_geometric.data.InMemoryDataset

property raw_file_names(*self*)

property processed_file_names(*self*)

download(*self*)

process(*self*)

class cogdl.datasets.pyg_strategies_data.**MoleculeDataset**(*data_type='unsupervised'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *empty=False*)

Bases: torch_geometric.data.InMemoryDataset

get(*self*, *idx*)

property raw_file_names(*self*)

property processed_file_names(*self*)

download(*self*)

process(*self*)

class cogdl.datasets.pyg_strategies_data.**BACEDataset**(*transform=None*, *pre_transform=None*, *pre_filter=None*, *empty=False*)

Bases: torch_geometric.data.InMemoryDataset

get(*self*, *idx*)

property raw_file_names(*self*)

property processed_file_names(*self*)

download(*self*)

process(*self*)

class cogdl.datasets.pyg_strategies_data.**BBBPDataset**(*transform=None*, *pre_transform=None*, *pre_filter=None*, *empty=False*)

Bases: torch_geometric.data.InMemoryDataset

get(*self*, *idx*)

property raw_file_names(*self*)

property processed_file_names(*self*)

download(*self*)

process(*self*)

Package Contents

Classes

Dataset	Dataset base class for creating graph datasets.

Functions

register_dataset(name)	New dataset types can be added to cogdl with the *register_dataset()*
build_dataset(args)	
build_dataset_from_name(dataset)	

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

Bases: torch.utils.data.Dataset

Dataset base class for creating graph datasets. See here for the accompanying tutorial.

Args: 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)

property raw_file_names(*self*)

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

property processed_file_names(*self*)

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

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

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

abstract __len__(*self*)
The number of examples in the dataset.

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

property num_features(*self*)
Returns the number of features per node in the graph.

property raw_paths(*self*)
The filepaths to find in order to skip the download.

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

_download(*self*)

_process(*self*)

__getitem__(*self*, *idx*)
Gets the data object at index `idx` and transforms it (in case a `self.transform` is given).

__repr__(*self*)

cogdl.datasets.**pyg = False**

cogdl.datasets.**dgl_import = False**

cogdl.datasets.**DATASET_REGISTRY**

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():
    (...)
```

Args: name (str): the name of the dataset

cogdl.datasets.**dataset_name**

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

cogdl.datasets.**build_dataset_from_name**(*dataset*)

cogdl.layers

Submodules

cogdl.layers.gcc_module

Module Contents

Classes

GATLayer	
SELayer	Squeeze-and-excitation networks
ApplyNodeFunc	Update the node feature hv with MLP, BN and ReLU.
MLP	MLP with linear output
UnsupervisedGAT	
UnsupervisedMPNN	MPNN from
UnsupervisedGIN	GIN model
GraphEncoder	MPNN from

class cogdl.layers.gcc_module.**GATLayer**(*g*, *in_dim*, *out_dim*)
Bases: torch.nn.Module

edge_attention(*self*, *edges*)

message_func(*self*, *edges*)

reduce_func(*self*, *nodes*)

forward(*self*, *h*)

class cogdl.layers.gcc_module.**SELayer**(*in_channels*, *se_channels*)
Bases: torch.nn.Module

Squeeze-and-excitation networks

forward(*self*, *x*)

class cogdl.layers.gcc_module.**ApplyNodeFunc**(*mlp*, *use_selayer*)
Bases: torch.nn.Module

Update the node feature hv with MLP, BN and ReLU.

forward(*self*, *h*)

class cogdl.layers.gcc_module.**MLP**(*num_layers*, *input_dim*, *hidden_dim*, *output_dim*, *use_selayer*)
Bases: torch.nn.Module

MLP with linear output

forward(*self*, *x*)

class cogdl.layers.gcc_module.**UnsupervisedGAT**(*node_input_dim*, *node_hidden_dim*, *edge_input_dim*, *num_layers*, *num_heads*)
Bases: torch.nn.Module

forward(*self*, *g*, *n_feat*, *e_feat*)

class cogdl.layers.gcc_module.**UnsupervisedMPNN**(*output_dim=32*, *node_input_dim=32*, *node_hidden_dim=32*, *edge_input_dim=32*, *edge_hidden_dim=32*, *num_step_message_passing=6*, *lstm_as_gate=False*)

Bases: torch.nn.Module

MPNN from Neural Message Passing for Quantum Chemistry

node_input_dim [int] Dimension of input node feature, default to be 15.

edge_input_dim [int] Dimension of input edge feature, default to be 15.

output_dim [int] Dimension of prediction, default to be 12.

node_hidden_dim [int] Dimension of node feature in hidden layers, default to be 64.

edge_hidden_dim [int] Dimension of edge feature in hidden layers, default to be 128.

num_step_message_passing [int] Number of message passing steps, default to be 6.

num_step_set2set [int] Number of set2set steps

num_layer_set2set [int] Number of set2set layers

forward(*self*, *g*, *n_feat*, *e_feat*)

Predict molecule labels

g [DGLGraph] Input DGLGraph for molecule(s)

n_feat [tensor of dtype float32 and shape (B1, D1)] Node features. B1 for number of nodes and D1 for the node feature size.

e_feat [tensor of dtype float32 and shape (B2, D2)] Edge features. B2 for number of edges and D2 for the edge feature size.

res : Predicted labels

class cogdl.layers.gcc_module.**UnsupervisedGIN**(*num_layers*, *num_mlp_layers*, *input_dim*, *hidden_dim*, *output_dim*, *final_dropout*, *learn_eps*, *graph_pooling_type*, *neighbor_pooling_type*, *use_selayer*)

Bases: torch.nn.Module

GIN model

forward(*self*, *g*, *h*, *efeat*)

class cogdl.layers.gcc_module.**GraphEncoder**(*positional_embedding_size=32*, *max_node_freq=8*, *max_edge_freq=8*, *max_degree=128*, *freq_embedding_size=32*, *degree_embedding_size=32*, *output_dim=32*, *node_hidden_dim=32*, *edge_hidden_dim=32*, *num_layers=6*, *num_heads=4*, *num_step_set2set=6*, *num_layer_set2set=3*, *norm=False*, *gnn_model='mpnn'*, *degree_input=False*, *lstm_as_gate=False*)

Bases: torch.nn.Module

MPNN from Neural Message Passing for Quantum Chemistry

node_input_dim [int] Dimension of input node feature, default to be 15.

edge_input_dim [int] Dimension of input edge feature, default to be 15.

output_dim [int] Dimension of prediction, default to be 12.

node_hidden_dim [int] Dimension of node feature in hidden layers, default to be 64.

edge_hidden_dim [int] Dimension of edge feature in hidden layers, default to be 128.

num_step_message_passing [int] Number of message passing steps, default to be 6.

num_step_set2set [int] Number of set2set steps

num_layer_set2set [int] Number of set2set layers

forward(*self*, *g*, *return_all_outputs=False*)

Predict molecule labels

g [DGLGraph] Input DGLGraph for molecule(s)

n_feat [tensor of dtype float32 and shape (B1, D1)] Node features. B1 for number of nodes and D1 for the node feature size.

e_feat [tensor of dtype float32 and shape (B2, D2)] Edge features. B2 for number of edges and D2 for the edge feature size.

res : Predicted labels

cogdl.layers.gpt_gnn_module

Module Contents

Classes

Graph	
HGTConv	
RelTemporalEncoding	Implement the Temporal Encoding (Sinusoid) function.
GeneralConv	
GNN	
GPT_GNN	
Classifier	
Matcher	Matching between a pair of nodes to conduct link prediction.
RNNModel	Container module with an encoder, a recurrent module, and a decoder.

Functions

args_print(args)	
dcg_at_k(r, k)	
ndcg_at_k(r, k)	
mean_reciprocal_rank(rs)	
normalize(mx)	Row-normalize sparse matrix
sparse_mx_to_torch_sparse_tensor(sparse_mx)	Convert a scipy sparse matrix to a torch sparse tensor.
randint()	
feature_OAG(layer_data, graph)	
feature_reddit(layer_data, graph)	
load_gnn(_dict)	
defaultDictDict()	
defaultDictList()	
defaultDictInt()	
defaultDictDictInt()	
defaultDictDictDictInt()	
defaultDictDictDictDictInt()	
defaultDictDictDictDictDictInt()	
sample_subgraph(graph, time_range, sampled_depth=2, sampled_number=8, inp=None, feature_extractor=feature_OAG)	Sample Sub-Graph based on the connection of other nodes with currently sampled nodes
to_torch(feature, time, edge_list, graph)	Transform a sampled sub-graph into pytorch Tensor
preprocess_dataset(dataset) → cogdl.layers.gpt_gnn_module.Graph	

cogdl.layers.gpt_gnn_module.**args_print**(*args*)

cogdl.layers.gpt_gnn_module.**dcg_at_k**(*r*, *k*)

cogdl.layers.gpt_gnn_module.**ndcg_at_k**(*r*, *k*)

cogdl.layers.gpt_gnn_module.**mean_reciprocal_rank**(*rs*)

cogdl.layers.gpt_gnn_module.**normalize**(*mx*)
Row-normalize sparse matrix

cogdl.layers.gpt_gnn_module.**sparse_mx_to_torch_sparse_tensor**(*sparse_mx*)
Convert a scipy sparse matrix to a torch sparse tensor.

cogdl.layers.gpt_gnn_module.**randint**()

cogdl.layers.gpt_gnn_module.**feature_OAG**(*layer_data*, *graph*)

cogdl.layers.gpt_gnn_module.**feature_reddit**(*layer_data*, *graph*)

cogdl.layers.gpt_gnn_module.**load_gnn**(*_dict*)

cogdl.layers.gpt_gnn_module.**defaultDictDict**()

cogdl.layers.gpt_gnn_module.**defaultDictList**()

cogdl.layers.gpt_gnn_module.**defaultDictInt**()

cogdl.layers.gpt_gnn_module.**defaultDictDictInt**()

cogdl.layers.gpt_gnn_module.**defaultDictDictDictInt**()

cogdl.layers.gpt_gnn_module.**defaultDictDictDictDictInt**()

cogdl.layers.gpt_gnn_module.**defaultDictDictDictDictDictInt**()

class cogdl.layers.gpt_gnn_module.**Graph**

node_feature
edge_list: index the adjacancy matrix (time) by <target_type, source_type, relation_type, target_id, source_id>

add_node(*self*, *node*)

add_edge(*self*, *source_node*, *target_node*, *time=None*, *relation_type=None*, *directed=True*)

update_node(*self*, *node*)

get_meta_graph(*self*)

get_types(*self*)

cogdl.layers.gpt_gnn_module.**sample_subgraph**(*graph*, *time_range*, *sampled_depth=2*, *sampled_number=8*, *inp=None*, *feature_extractor=feature_OAG*)
Sample Sub-Graph based on the connection of other nodes with currently sampled nodes We maintain budgets for each node type, indexed by <node_id, time>. Currently sampled nodes are stored in layer_data. After nodes are sampled, we construct the sampled adjacancy matrix.

cogdl.layers.gpt_gnn_module.**to_torch**(*feature*, *time*, *edge_list*, *graph*)
Transform a sampled sub-graph into pytorch Tensor node_dict: {node_type: <node_number, node_type_ID>} node_number is used to trace back the nodes in original graph. edge_dict: {edge_type: edge_type_ID}

class cogdl.layers.gpt_gnn_module.**HGTConv**(*in_dim*, *out_dim*, *num_types*, *num_relations*, *n_heads*, *dropout=0.2*, *use_norm=True*, *use_RTE=True*, ***kwargs*)
Bases: torch_geometric.nn.conv.MessagePassing

forward(*self*, *node_inp*, *node_type*, *edge_index*, *edge_type*, *edge_time*)

message(*self*, *edge_index_i*, *node_inp_i*, *node_inp_j*, *node_type_i*, *node_type_j*, *edge_type*, *edge_time*)
j: source, i: target; <j, i>

update(*self*, *aggr_out*, *node_inp*, *node_type*)
Step 3: Target-specific Aggregation x = W[node_type] * gelu(Agg(x)) + x

__repr__(*self*)

class cogdl.layers.gpt_gnn_module.**RelTemporalEncoding**(*n_hid*, *max_len=240*, *dropout=0.2*)

Bases: torch.nn.Module

Implement the Temporal Encoding (Sinusoid) function.

forward(*self*, *x*, *t*)

class cogdl.layers.gpt_gnn_module.**GeneralConv**(*conv_name*, *in_hid*, *out_hid*, *num_types*, *num_relations*, *n_heads*, *dropout*, *use_norm=True*, *use_RTE=True*)

Bases: torch.nn.Module

forward(*self*, *meta_xs*, *node_type*, *edge_index*, *edge_type*, *edge_time*)

class cogdl.layers.gpt_gnn_module.**GNN**(*in_dim*, *n_hid*, *num_types*, *num_relations*, *n_heads*, *n_layers*, *dropout=0.2*, *conv_name='hgt'*, *prev_norm=False*, *last_norm=False*, *use_RTE=True*)

Bases: torch.nn.Module

forward(*self*, *node_feature*, *node_type*, *edge_time*, *edge_index*, *edge_type*)

class cogdl.layers.gpt_gnn_module.**GPT_GNN**(*gnn*, *rem_edge_list*, *attr_decoder*, *types*, *neg_samp_num*, *device*, *neg_queue_size=0*)

Bases: torch.nn.Module

neg_sample(*self*, *souce_node_list*, *pos_node_list*)

forward(*self*, *node_feature*, *node_type*, *edge_time*, *edge_index*, *edge_type*)

link_loss(*self*, *node_emb*, *rem_edge_list*, *ori_edge_list*, *node_dict*, *target_type*, *use_queue=True*, *update_queue=False*)

text_loss(*self*, *reps*, *texts*, *w2v_model*, *device*)

feat_loss(*self*, *reps*, *out*)

class cogdl.layers.gpt_gnn_module.**Classifier**(*n_hid*, *n_out*)

Bases: torch.nn.Module

forward(*self*, *x*)

__repr__(*self*)

class cogdl.layers.gpt_gnn_module.**Matcher**(*n_hid*, *n_out*, *temperature=0.1*)

Bases: torch.nn.Module

Matching between a pair of nodes to conduct link prediction. Use multi-head attention as matching model.

forward(*self*, *x*, *ty*, *use_norm=True*)

__repr__(*self*)

class cogdl.layers.gpt_gnn_module.**RNNModel**(*n_word*, *ninp*, *nhid*, *nlayers*, *dropout=0.2*)

Bases: torch.nn.Module

Container module with an encoder, a recurrent module, and a decoder.

forward(*self*, *inp*, *hidden=None*)

from_w2v(*self*, *w2v*)

cogdl.layers.gpt_gnn_module.**preprocess_dataset**(*dataset*) → *cogdl.layers.gpt_gnn_module.Graph*

cogdl.layers.link_prediction_module

Module Contents

Classes

DistMultLayer	
ConvELayer	
GNNLinkPredict	

Functions

cal_mrr(embedding, rel_embedding, edge_index, edge_type, scoring, protocol='raw', batch_size=1000, hits=[])	
sampling_edge_uniform(edge_index, edge_types, edge_set, sampling_rate, num_rels, label_smoothing=0.0, num_entities=1)	Args:
get_rank(scores, target)	
get_raw_rank(heads, tails, rels, embedding, rel_embedding, batch_size, scoring)	
get_filtered_rank(heads, tails, rels, embedding, rel_embedding, batch_size, seen_data)	

cogdl.layers.link_prediction_module.**cal_mrr**(*embedding*, *rel_embedding*, *edge_index*, *edge_type*, *scoring*, *protocol='raw'*, *batch_size=1000*, *hits=[]*)

class cogdl.layers.link_prediction_module.**DistMultLayer**

Bases: torch.nn.Module

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

predict(*self*, *sub_emb*, *obj_emb*, *rel_emb*)

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

Bases: torch.nn.Module

concat(*self*, *ent*, *rel*)

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

predict(*self*, *sub_emb*, *obj_emb*, *rel_emb*)

class cogdl.layers.link_prediction_module.**GNNLinkPredict**(*score_func*, *dim*)

Bases: torch.nn.Module

forward(*self*, *edge_index*, *edge_type*)

get_score(*self*, *heads*, *tails*, *rels*)

get_edge_set(*self*, *edge_index*, *edge_types*)

_loss(*self*, *head_embed*, *tail_embed*, *rel_embed*, *labels*)

_regularization(*self*, *embs*)

cogdl.layers.link_prediction_module.**sampling_edge_uniform**(*edge_index*, *edge_types*, *edge_set*, *sampling_rate*, *num_rels*, *label_smoothing=0.0*, *num_entities=1*)

Args: 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_edges: 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

cogdl.layers.link_prediction_module.**get_rank**(*scores*, *target*)

cogdl.layers.link_prediction_module.**get_raw_rank**(*heads*, *tails*, *rels*, *embedding*, *rel_embedding*, *batch_size*, *scoring*)

cogdl.layers.link_prediction_module.**get_filtered_rank**(*heads*, *tails*, *rels*, *embedding*, *rel_embedding*, *batch_size*, *seen_data*)

cogdl.layers.maggregator

Module Contents

Classes

MeanAggregator

class cogdl.layers.maggregator.**MeanAggregator**(*in_channels*, *out_channels*, *improved=False*, *cached=False*, *bias=True*)

Bases: `torch.nn.Module`

static norm(*x*, *edge_index*)

forward(*self*, *x*, *edge_index*, *edge_weight=None*, *bias=True*)

update(*self*, *aggr_out*)

__repr__(*self*)

cogdl.layers.mixhop_layer

Module Contents

Classes

MixHopLayer	

class cogdl.layers.mixhop_layer.**MixHopLayer**(*num_features*, *adj_pows*, *dim_per_pow*)
Bases: torch.nn.Module

reset_parameters(*self*)

adj_pow_x(*self*, *x*, *adj*, *p*)

forward(*self*, *x*, *edge_index*)

cogdl.layers.mixhop_layer.**layer**

cogdl.layers.prone_module

Module Contents

Classes

HeatKernel	
HeatKernelApproximation	
Gaussian	
PPR	applying sparsification to accelerate computation
SignalRescaling	• rescale signal of each node according to the degree of the node:
ProNE	
NodeAdaptiveEncoder	• shrink negative values in signal/feature matrix

Functions

propagate(mx, emb, stype, space=None)

get_embedding_dense(matrix, dimension)

class cogdl.layers.prone_module.**HeatKernel**(*t=0.5*, *theta0=0.6*, *theta1=0.4*)
Bases: object

prop_adjacency(*self*, *mx*)

prop(*self*, *mx*, *emb*)

class cogdl.layers.prone_module.**HeatKernelApproximation**(*t=0.2*, *k=5*)
Bases: object

taylor(*self*, *mx*, *emb*)

chebyshev(*self*, *mx*, *emb*)

prop(*self*, *mx*, *emb*)

class cogdl.layers.prone_module.**Gaussian**(*mu=0.5*, *theta=1*, *rescale=False*, *k=3*)
Bases: object

prop(*self*, *mx*, *emb*)

class cogdl.layers.prone_module.**PPR**(*alpha=0.5*, *k=10*)
Bases: object

applying sparsification to accelerate computation

prop(*self*, *mx*, *emb*)

class cogdl.layers.prone_module.**SignalRescaling**
Bases: object

- rescale signal of each node according to the degree of the node:
- sigmoid(degree)
- sigmoid(1/degree)

prop(*self*, *mx*, *emb*)

class cogdl.layers.prone_module.**ProNE**
Bases: object

__call__(*self*, *A*, *a*, *order=10*, *mu=0.1*, *s=0.5*)

class cogdl.layers.prone_module.**NodeAdaptiveEncoder**
Bases: object

- shrink negative values in signal/feature matrix
- no learning

static prop(*signal*)

cogdl.layers.prone_module.**propagate**(*mx*, *emb*, *stype*, *space=None*)

cogdl.layers.prone_module.**get_embedding_dense**(*matrix*, *dimension*)

cogdl.layers.se_layer

Module Contents

Classes

SELayer	Squeeze-and-excitation networks

class cogdl.layers.se_layer.**SELayer**(*in_channels*, *se_channels*)
Bases: torch.nn.Module

Squeeze-and-excitation networks

forward(*self*, *x*)

cogdl.layers.srgcn_module

Module Contents

Classes

NodeAttention
EdgeAttention
Identity
PPR
HeatKernel
NormIdentity
RowUniform
RowSoftmax
ColumnUniform
SymmetryNorm

Functions

act_attention(attn_type)
act_normalization(norm_type)
act_map(act)

class cogdl.layers.srgcn_module.**NodeAttention**(*in_feat*)
Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*)

class cogdl.layers.srgcn_module.**EdgeAttention**(*in_feat*)
Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*)

class cogdl.layers.srgcn_module.**Identity**(*in_feat*)
Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*)

class cogdl.layers.srgcn_module.**PPR**(*in_feat*)
Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*)

class cogdl.layers.srgcn_module.**HeatKernel**(*in_feat*)
Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*)

cogdl.layers.srgcn_module.**act_attention**(*attn_type*)

class cogdl.layers.srgcn_module.**NormIdentity**
Bases: torch.nn.Module

forward(*self*, *edge_index*, *edge_attr*, *N*)

class cogdl.layers.srgcn_module.**RowUniform**
Bases: torch.nn.Module

forward(*self*, *edge_index*, *edge_attr*, *N*)

class cogdl.layers.srgcn_module.**RowSoftmax**
Bases: torch.nn.Module

forward(*self*, *edge_index*, *edge_attr*, *N*)

class cogdl.layers.srgcn_module.**ColumnUniform**
Bases: torch.nn.Module

forward(*self*, *edge_index*, *edge_attr*, *N*)

class cogdl.layers.srgcn_module.**SymmetryNorm**
Bases: torch.nn.Module

forward(*self*, *edge_index*, *edge_attr*, *N*)

cogdl.layers.srgcn_module.**act_normalization**(*norm_type*)

cogdl.layers.srgcn_module.**act_map**(*act*)

cogdl.layers.strategies_layers

Module Contents

Classes

GINConv
GNN
GNNPred
Pretrainer
Discriminator
InfoMaxTrainer
ContextPredictTrainer
MaskTrainer
SupervisedTrainer
Finetuner

class cogdl.layers.strategies_layers.**GINConv**(*hidden_size*, *input_layer=None*, *edge_emb=None*, *edge_encode=None*, *pooling='sum'*, *feature_concat=False*)

Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*, *self_loop_index=None*, *self_loop_type=None*)

aggr(*self*, *x*, *edge_index*, *num_nodes*)

class cogdl.layers.strategies_layers.**GNN**(*num_layers*, *hidden_size*, *JK='last'*, *dropout=0.5*, *input_layer=None*, *edge_encode=None*, *edge_emb=None*, *num_atom_type=None*, *num_chirality_tag=None*, *concat=False*)

Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*, *self_loop_index=None*, *self_loop_type=None*)

class cogdl.layers.strategies_layers.**GNNPred**(*num_layers*, *hidden_size*, *num_tasks*, *JK='last'*, *dropout=0*, *graph_pooling='mean'*, *input_layer=None*, *edge_encode=None*, *edge_emb=None*, *num_atom_type=None*, *num_chirality_tag=None*, *concat=True*)

Bases: torch.nn.Module

load_from_pretrained(*self*, *path*)

forward(*self*, *data*, *self_loop_index*, *self_loop_type*)

pool(*self*, *x*, *batch*)

class cogdl.layers.strategies_layers.**Pretrainer**(*args*, *transform=None*)
Bases: torch.nn.Module

get_dataset(*self*, *dataset_name*, *transform=None*)

fit(*self*)

class cogdl.layers.strategies_layers.**Discriminator**(*hidden_size*)
Bases: torch.nn.Module

reset_parameters(*self*)

forward(*self*, *x*, *summary*)

class cogdl.layers.strategies_layers.**InfoMaxTrainer**(*args*)
Bases: *cogdl.layers.strategies_layers.Pretrainer*

static add_args(*parser*)

_train_step(*self*)

class cogdl.layers.strategies_layers.**ContextPredictTrainer**(*args*)
Bases: *cogdl.layers.strategies_layers.Pretrainer*

static add_args(*parser*)

_train_step(*self*)

get_cbow_pred(*self*, *overlapped_rep*, *overlapped_context*, *neighbor_rep*)

get_skipgram_pred(*self*, *overlapped_rep*, *overlapped_context_size*, *neighbor_rep*)

class cogdl.layers.strategies_layers.**MaskTrainer**(*args*)
Bases: *cogdl.layers.strategies_layers.Pretrainer*

static add_args(*parser*)

_train_step(*self*)

class cogdl.layers.strategies_layers.**SupervisedTrainer**(*args*)
Bases: *cogdl.layers.strategies_layers.Pretrainer*

static add_args(*parser*)

split_data(*self*)

_train_step(*self*)

class cogdl.layers.strategies_layers.**Finetuner**(*args*)
Bases: *cogdl.layers.strategies_layers.Pretrainer*

static add_args(*parser*)

build_model(*self*, *args*)

split_data(*self*)

_train_step(*self*)

_test_step(*self*, *split='val'*)

fit(*self*)

Package Contents

Classes

MeanAggregator	
SELayer	Squeeze-and-excitation networks
MixHopLayer	

class cogdl.layers.**MeanAggregator**(*in_channels*, *out_channels*, *improved=False*, *cached=False*, *bias=True*)

Bases: torch.nn.Module

static norm(*x*, *edge_index*)

forward(*self*, *x*, *edge_index*, *edge_weight=None*, *bias=True*)

update(*self*, *aggr_out*)

__repr__(*self*)

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

Bases: torch.nn.Module

Squeeze-and-excitation networks

forward(*self*, *x*)

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

Bases: torch.nn.Module

reset_parameters(*self*)

adj_pow_x(*self*, *x*, *adj*, *p*)

forward(*self*, *x*, *edge_index*)

cogdl.models

Subpackages

cogdl.models.emb

Submodules

cogdl.models.emb.complex

Module Contents

Classes

ComplEx	the implementation of ComplEx model from the paper *"Complex Embeddings for Simple Link Prediction"<http://proceedings.mlr.press/v48/trouillon16.pdf>*

class cogdl.models.emb.complex.**ComplEx**(*nentity*, *nrelation*, *hidden_dim*, *gamma*, *double_entity_embedding=False*, *double_relation_embedding=False*)

Bases: *cogdl.models.emb.knowledge_base.KGEModel*

the implementation of ComplEx model from the paper *"Complex Embeddings for Simple Link Prediction"<http://proceedings.mlr.press/v48/trouillon16.pdf>* borrowed from *KnowledgeGraphEmbedding<https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding>*

score(*self*, *head*, *relation*, *tail*, *mode*)

cogdl.models.emb.deepwalk

Module Contents

Classes

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

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

Bases: *cogdl.models.BaseModel*

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

Args: 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*)
Add model-specific arguments to the parser.

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

train(*self*, *G*)

_walk(*self*, *start_node*, *walk_length*)

_simulate_walks(*self*, *walk_length*, *num_walks*)

cogdl.models.emb.dgk

Module Contents

Classes

DeepGraphKernel	The Hin2vec model from the ``"Deep Graph Kernels"

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

Bases: *cogdl.models.BaseModel*

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

Args: 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. epoch (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(*cls*, *args*)
Build a new model instance.

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

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

forward(*self*, *graphs*, ***kwargs*)

save_embedding(*self*, *output_path*)

cogdl.models.emb.distmult

Module Contents

Classes

DistMult	The DistMult model from the ICLR 2015 paper ``"EMBEDDING ENTITIES AND RELATIONS FOR LEARNING AND INFERENCE IN KNOWLEDGE BASES"

class cogdl.models.emb.distmult.**DistMult**(*nentity*, *nrelation*, *hidden_dim*, *gamma*, *double_entity_embedding=False*, *double_relation_embedding=False*)

Bases: *cogdl.models.emb.knowledge_base.KGEModel*

The DistMult model from the ICLR 2015 paper *"EMBEDDING ENTITIES AND RELATIONS FOR LEARNING AND INFERENCE IN KNOWLEDGE BASES" <https://www.microsoft.com/en-us/research/wp-content/uploads/2016/02/ICLR2015_updated.pdf>* borrowed from *KnowledgeGraphEmbedding<https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding>*

score(*self*, *head*, *relation*, *tail*, *mode*)

cogdl.models.emb.dngr

Module Contents

Classes

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

class cogdl.models.emb.dngr.**DNGR_layer**(*num_node*, *hidden_size1*, *hidden_size2*)

Bases: torch.nn.Module

forward(*self*, *x*)

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

Bases: *cogdl.models.BaseModel*

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

Args: 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. max_epoch (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(*cls*, *args*)

Build a new model instance.

scale_matrix(*self*, *mat*)

random_surfing(*self*, *adj_matrix*)

get_ppmi_matrix(*self*, *mat*)

get_denoised_matrix(*self*, *mat*)

get_emb(*self*, *matrix*)

train(*self*, *G*)

cogdl.models.emb.gatne

Module Contents

Classes

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

continues on next page

Table 49 – continued from previous page

GATNEModel
NSLoss
RWGraph

Functions

get_G_from_edges(edges)
generate_pairs(all_walks, vocab, window_size=5)
generate_vocab(all_walks)
get_batches(pairs, neighbors, batch_size)
generate_walks(network_data, num_walks, walk_length, schema=None)

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

Bases: *cogdl.models.BaseModel*

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

Args: 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. epoch (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 ",", while each node type are connected with "-" in each metapath. For example:"0-1-0,0-1-2-1-0"

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

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

train(*self*, *network_data*)

class cogdl.models.emb.gatne.**GATNEModel**(*num_nodes*, *embedding_size*, *embedding_u_size*, *edge_type_count*, *dim_a*)

Bases: torch.nn.Module

reset_parameters(*self*)

forward(*self*, *train_inputs*, *train_types*, *node_neigh*)

class cogdl.models.emb.gatne.**NSLoss**(*num_nodes*, *num_sampled*, *embedding_size*)

Bases: torch.nn.Module

reset_parameters(*self*)

forward(*self*, *input*, *embs*, *label*)

class cogdl.models.emb.gatne.**RWGraph**(*nx_G*, *node_type=None*)

walk(*self*, *walk_length*, *start*, *schema=None*)

simulate_walks(*self*, *num_walks*, *walk_length*, *schema=None*)

cogdl.models.emb.gatne.**get_G_from_edges**(*edges*)

cogdl.models.emb.gatne.**generate_pairs**(*all_walks*, *vocab*, *window_size=5*)

cogdl.models.emb.gatne.**generate_vocab**(*all_walks*)

cogdl.models.emb.gatne.**get_batches**(*pairs*, *neighbors*, *batch_size*)

cogdl.models.emb.gatne.**generate_walks**(*network_data*, *num_walks*, *walk_length*, *schema=None*)

cogdl.models.emb.graph2vec

Module Contents

Classes

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

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

Bases: *cogdl.models.BaseModel*

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

Args: 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. epoch (int) : The max epoches in training step. lr (float) : Learning rate in doc2vec.

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

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

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

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

forward(*self*, *graphs*, ***kwargs*)

save_embedding(*self*, *output_path*)

cogdl.models.emb.grarep

Module Contents

Classes

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

class cogdl.models.emb.grarep.**GraRep**(*dimension*, *step*)

Bases: *cogdl.models.BaseModel*

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

Args: 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(*cls*, *args*)

Build a new model instance.

train(*self*, *G*)

_get_embedding(*self*, *matrix*, *dimension*)

cogdl.models.emb.hin2vec

Module Contents

Classes

Hin2vec_layer	
RWgraph	
Hin2vec	The Hin2vec model from the `"HIN2Vec: Explore Meta-paths in Heterogeneous Information Networks for Representation Learning"

class cogdl.models.emb.hin2vec.**Hin2vec_layer**(*num_node*, *num_relation*, *hidden_size*, *cpu*)

Bases: torch.nn.Module

regulartion(*self*, *embr*)

forward(*self*, *x*, *y*, *r*, *l*)

get_emb(*self*)

class cogdl.models.emb.hin2vec.**RWgraph**(*nx_G*, *node_type=None*)

_walk(*self*, *start_node*, *walk_length*)

_simulate_walks(*self*, *walk_length*, *num_walks*)

data_preparation(*self*, *walks*, *hop*, *negative*)

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

Bases: *cogdl.models.BaseModel*

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

Args: 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(*cls*, *args*)
Build a new model instance.

train(*self*, *G*, *node_type*)

cogdl.models.emb.hope

Module Contents

Classes

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

class cogdl.models.emb.hope.**HOPE**(*dimension*, *beta*)

Bases: *cogdl.models.BaseModel*

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

Args: 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(*cls*, *args*)
Build a new model instance.

train(*self*, *G*)
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

_get_embedding(*self*, *matrix*, *dimension*)

cogdl.models.emb.knowledge_base

Module Contents

Classes

KGEModel	

class cogdl.models.emb.knowledge_base.**KGEModel**(*nentity*, *nrelation*, *hidden_dim*, *gamma*, *double_entity_embedding=False*, *double_relation_embedding=False*)

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *sample*, *mode='single'*)
Forward function that calculate the score of a batch of triples. In the 'single' mode, sample is a batch of triple. In the 'head-batch' or 'tail-batch' mode, sample consists two part. The first part is usually the positive sample. And the second part is the entities in the negative samples. Because negative samples and positive samples usually share two elements in their triple ((head, relation) or (relation, tail)).

abstract score(*self*, *head*, *relation*, *tail*, *mode*)

static train_step(*model*, *optimizer*, *train_iterator*, *args*)
A single train step. Apply back-propation and return the loss

static test_step(*model*, *test_triples*, *all_true_triples*, *args*)
Evaluate the model on test or valid datasets

cogdl.models.emb.line

Module Contents

Classes

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

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

Bases: *cogdl.models.BaseModel*

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

Args: 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 negative 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, while 3

means both of them (each of them having dimension/2 node representation).

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

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

train(*self*, *G*)

_update(*self*, *vec_u*, *vec_v*, *vec_error*, *label*)

_train_line(*self*, *order*)

cogdl.models.emb.metapath2vec

Module Contents

Classes

Metapath2vec	The Metapath2vec model from the `"metapath2vec: Scalable Representation

class cogdl.models.emb.metapath2vec.**Metapath2vec**(*dimension*, *walk_length*, *walk_num*, *window_size*, *worker*, *iteration*, *schema*)

Bases: *cogdl.models.BaseModel*

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

Args: 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 ",", while each node type are connected with "-" in each metapath. For example:"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(*cls*, *args*)
Build a new model instance.

train(*self*, *G*, *node_type*)

_walk(*self*, *start_node*, *walk_length*, *schema=None*)

_simulate_walks(*self*, *walk_length*, *num_walks*, *schema='No'*)

cogdl.models.emb.netmf

Module Contents

Classes

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

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

Bases: *cogdl.models.BaseModel*

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

Args: 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(*cls*, *args*)

Build a new model instance.

train(*self*, *G*)

_compute_deepwalk_matrix(*self*, *A*, *window*, *b*)

_approximate_normalized_laplacian(*self*, *A*, *rank*, *which='LA'*)

_deepwalk_filter(*self*, *evals*, *window*)

_approximate_deepwalk_matrix(*self*, *evals*, *D_rt_invU*, *window*, *vol*, *b*)

cogdl.models.emb.netsmf

Module Contents

Classes

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

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

Bases: *cogdl.models.BaseModel*

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

Args: 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(*cls*, *args*)
Build a new model instance.

train(*self*, *G*)

_get_embedding_rand(*self*, *matrix*)

_path_sampling(*self*, *u*, *v*, *r*)

_random_walk_matrix(*self*, *pid*)

cogdl.models.emb.node2vec

Module Contents

Classes

Node2vec	The node2vec model from the `"node2vec: Scalable feature learning for networks"

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

Bases: *cogdl.models.BaseModel*

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

Args: 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(*cls*, *args*)
Build a new model instance.

train(*self*, *G*)

_node2vec_walk(*self*, *walk_length*, *start_node*)

_simulate_walks(*self*, *num_walks*, *walk_length*)

_get_alias_edge(*self*, *src*, *dst*)

_preprocess_transition_probs(*self*)

cogdl.models.emb.prone

Module Contents

Classes

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

class cogdl.models.emb.prone.**ProNE**(*dimension*, *step*, *mu*, *theta*)

Bases: *cogdl.models.BaseModel*

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

Args: 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(*cls*, *args*)

Build a new model instance.

train(*self*, *G*)

_get_embedding_rand(*self*, *matrix*)

_get_embedding_dense(*self*, *matrix*, *dimension*)

_pre_factorization(*self*, *tran*, *mask*)

_chebyshev_gaussian(*self*, *A*, *a*, *order=5*, *mu=0.5*, *s=0.2*, *plus=False*, *nn=False*)

cogdl.models.emb.pte

Module Contents

Classes

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

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

Bases: *cogdl.models.BaseModel*

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

Args: 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 negative 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(*cls*, *args*)
Build a new model instance.

train(*self*, *G*, *node_type*)

_update(*self*, *vec_u*, *vec_v*, *vec_error*, *label*)

_train_line(*self*)

cogdl.models.emb.rotate

Module Contents

Classes

RotatE	Implementation of RotatE model from the paper `"RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space"

class cogdl.models.emb.rotate.**RotatE**(*nentity*, *nrelation*, *hidden_dim*, *gamma*, *double_entity_embedding=False*, *double_relation_embedding=False*)

Bases: *cogdl.models.emb.knowledge_base.KGEModel*

Implementation of RotatE model from the paper *"RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space" <https://openreview.net/forum?id=HkgEQnRqYQ>*. borrowed from *KnowledgeGraphEmbedding<https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding>*

score(*self*, *head*, *relation*, *tail*, *mode*)

cogdl.models.emb.sdne

Module Contents

Classes

SDNE_layer	
SDNE	The SDNE model from the `"Structural Deep Network Embedding"

class cogdl.models.emb.sdne.**SDNE_layer**(*num_node*, *hidden_size1*, *hidden_size2*, *droput*, *alpha*, *beta*, *nu1*, *nu2*)

Bases: `torch.nn.Module`

forward(*self*, *adj_mat*, *l_mat*)

get_emb(*self*, *adj*)

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

Bases: *cogdl.models.BaseModel*

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

Args: 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. max_epoch (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(*cls*, *args*)
Build a new model instance.

train(*self*, *G*)

cogdl.models.emb.spectral

Module Contents

Classes

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

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

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

Args: hidden_size (int) : The dimension of node representation.

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

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

train(*self*, *G*)

cogdl.models.emb.transe

Module Contents

Classes

TransE	The TransE model from paper `"Translating Embeddings for Modeling Multi-relational Data"

class cogdl.models.emb.transe.**TransE**(*nentity*, *nrelation*, *hidden_dim*, *gamma*, *double_entity_embedding=False*, *double_relation_embedding=False*)

Bases: *cogdl.models.emb.knowledge_base.KGEModel*

The TransE model from paper *"Translating Embeddings for Modeling Multi-relational Data" <http://papers.nips.cc/paper/5071-translating-embeddings-for-modeling-multi-relational-data.pdf>* borrowed from *KnowledgeGraphEmbedding<https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding>*

score(*self*, *head*, *relation*, *tail*, *mode*)

cogdl.models.nn

Submodules

cogdl.models.nn.asgcn

Module Contents

Classes

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

class cogdl.models.nn.asgcn.**GraphConvolution**(*in_features*, *out_features*, *bias=True*)

Bases: `torch.nn.Module`

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

reset_parameters(*self*)

forward(*self*, *input*, *adj*)

__repr__(*self*)

class cogdl.models.nn.asgcn.**ASGCN**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*, *sample_size*)

Bases: *cogdl.models.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*cls*, *args*)

Build a new model instance.

reset_parameters(*self*)

set_adj(*self*, *edge_index*, *num_nodes*)

compute_adjlist(*self*, *sp_adj*, *max_degree=32*)

Transfer sparse adjacent matrix to adj-list format

from_adjlist(*self*, *adj*)

Transfer adj-list format to sparsetensor

_sample_one_layer(*self*, *x*, *adj*, *v*, *sample_size*)

sampling(*self*, *x*, *v*)

forward(*self*, *x*, *adj*)

cogdl.models.nn.compgcn

Module Contents

Classes

BasesRelEmbLayer	
CompGCNLayer	
CompGCN	
LinkPredictCompGCN	

Functions

com_mult(a, b)	Borrowed CompGCN	from	https://github.com/malllabiisc/
conj(a)	Borrowed CompGCN	from	https://github.com/malllabiisc/
ccorr(a, b)	Borrowed CompGCN	from	https://github.com/malllabiisc/

cogdl.models.nn.compgcn.**com_mult**(*a*, *b*)
Borrowed from https://github.com/malllabiisc/CompGCN

cogdl.models.nn.compgcn.**conj**(*a*)
Borrowed from https://github.com/malllabiisc/CompGCN

cogdl.models.nn.compgcn.**ccorr**(*a*, *b*)
Borrowed from https://github.com/malllabiisc/CompGCN

class cogdl.models.nn.compgcn.**BasesRelEmbLayer**(*num_bases*, *num_rels*, *in_feats*)
Bases: torch.nn.Module

reset_parameters(*self*)

forward(*self*)

class cogdl.models.nn.compgcn.**CompGCNLayer**(*in_feats*, *out_feats*, *num_rels*, *opn='mult'*, *num_bases=None*, *activation=lambda x: ...*, *dropout=0.0*, *bias=True*)
Bases: torch.nn.Module

get_param(*self*, *num_in*, *num_out*)

forward(*self*, *x*, *edge_index*, *edge_type*, *rel_embed=None*)

message_passing(*self*, *x*, *rel_embed*, *edge_index*, *edge_types*, *mode*, *edge_weight=None*)

rel_transform(*self*, *ent_embed*, *rel_embed*)

class cogdl.models.nn.compgcn.**CompGCN**(*num_entities*, *num_rels*, *num_bases*, *in_feats*, *hidden_size*, *out_feats*, *layers*, *dropout*, *activation*)
Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_types*)

class cogdl.models.nn.compgcn.**LinkPredictCompGCN**(*num_entities*, *num_rels*, *hidden_size*, *num_bases=0*, *layers=1*, *sampling_rate=0.01*, *score_func='conve'*, *penalty=0.001*, *dropout=0.0*, *lbl_smooth=0.1*)

Bases: *cogdl.layers.link_prediction_module.GNNLinkPredict*, *cogdl.models.BaseModel*

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

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

add_reverse_edges(*self*, *edge_index*, *edge_types*)

forward(*self*, *edge_index*, *edge_types*)

loss(*self*, *data*, *split='train'*)

predict(*self*, *edge_index*, *edge_types*)

cogdl.models.nn.dgi

Module Contents

Classes

GCN
AvgReadout
Discriminator
LogReg
LogRegTrainer
DGIModel
DGI

Functions

preprocess_features(features)	Row-normalize feature matrix and convert to tuple representation
normalize_adj(adj)	Symmetrically normalize adjacency matrix.
sparse_mx_to_torch_sparse_tensor(sparse_mx)	Convert a scipy sparse matrix to a torch sparse tensor.

class cogdl.models.nn.dgi.**GCN**(*in_ft*, *out_ft*, *act*, *bias=True*)
Bases: torch.nn.Module

weights_init(*self*, *m*)

forward(*self*, *seq*, *adj*, *sparse=False*)

class cogdl.models.nn.dgi.**AvgReadout**
Bases: torch.nn.Module

forward(*self*, *seq*, *msk*)

class cogdl.models.nn.dgi.**Discriminator**(*n_h*)
Bases: torch.nn.Module

weights_init(*self*, *m*)

forward(*self*, *c*, *h_pl*, *h_mi*, *s_bias1=None*, *s_bias2=None*)

class cogdl.models.nn.dgi.**LogReg**(*ft_in*, *nb_classes*)
Bases: torch.nn.Module

weights_init(*self*, *m*)

forward(*self*, *seq*)

class cogdl.models.nn.dgi.**LogRegTrainer**
Bases: object

train(*self*, *data*, *labels*, *opt*)

class cogdl.models.nn.dgi.**DGIModel**(*n_in*, *n_h*, *activation*)
Bases: torch.nn.Module

forward(*self*, *seq1*, *seq2*, *adj*, *sparse*, *msk*, *samp_bias1*, *samp_bias2*)

embed(*self*, *seq*, *adj*, *sparse*, *msk*)

cogdl.models.nn.dgi.**preprocess_features**(*features*)
Row-normalize feature matrix and convert to tuple representation

cogdl.models.nn.dgi.**normalize_adj**(*adj*)
Symmetrically normalize adjacency matrix.

cogdl.models.nn.dgi.**sparse_mx_to_torch_sparse_tensor**(*sparse_mx*)
Convert a scipy sparse matrix to a torch sparse tensor.

class cogdl.models.nn.dgi.**DGI**(*nfeat*, *nhid*, *nclass*, *max_epochs*)
Bases: *cogdl.models.BaseModel*

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

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

train(*self*, *data*)

cogdl.models.nn.dgl_gcc

Module Contents

Classes

NodeClassificationDataset	
GraphClassificationDataset	
GCC	

Functions

batcher()	
test_moco(train_loader, model, opt)	one epoch training for moco
eigen_decomposision(n, k, laplacian, hidden_size, retry)	
_add_undirected_graph_positional_embedding(g, hidden_size, retry=10)	
_rwr_trace_to_dgl_graph(g, seed, trace, positional_embedding_size, entire_graph=False)	

cogdl.models.nn.dgl_gcc.**batcher**()

cogdl.models.nn.dgl_gcc.**test_moco**(*train_loader*, *model*, *opt*)
one epoch training for moco

cogdl.models.nn.dgl_gcc.**eigen_decomposision**(*n*, *k*, *laplacian*, *hidden_size*, *retry*)

cogdl.models.nn.dgl_gcc.**_add_undirected_graph_positional_embedding**(*g*, *hidden_size*, *retry=10*)

cogdl.models.nn.dgl_gcc.**_rwr_trace_to_dgl_graph**(*g*, *seed*, *trace*, *positional_embedding_size*, *entire_graph=False*)

class cogdl.models.nn.dgl_gcc.**NodeClassificationDataset**(*data*, *rw_hops=64*, *subgraph_size=64*, *restart_prob=0.8*, *positional_embedding_size=32*, *step_dist=[1.0, 0.0, 0.0]*)

Bases: object

_create_dgl_graph(*self*, *data*)

__len__(*self*)

_convert_idx(*self*, *idx*)

__getitem__(*self*, *idx*)

class cogdl.models.nn.dgl_gcc.**GraphClassificationDataset**(*data*, *rw_hops=64*, *subgraph_size=64*, *restart_prob=0.8*, *positional_embedding_size=32*, *step_dist=[1.0, 0.0, 0.0]*)

Bases: *cogdl.models.nn.dgl_gcc.NodeClassificationDataset*

_convert_idx(*self*, *idx*)

class cogdl.models.nn.dgl_gcc.**GCC**(*load_path*)

Bases: *cogdl.models.BaseModel*

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

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

train(*self*, *data*)

cogdl.models.nn.disengcn

Module Contents

Classes

DisenGCNLayer	Implementation of "Disentangled Graph Convolutional Networks" <http://proceedings.mlr.press/v97/ma19a.html>.
DisenGCN	

class cogdl.models.nn.disengcn.**DisenGCNLayer**(*in_feats*, *out_feats*, *K*, *iterations*, *tau=1.0*, *activation='leaky_relu'*)

Bases: `torch.nn.Module`

Implementation of "Disentangled Graph Convolutional Networks" <http://proceedings.mlr.press/v97/ma19a.html>.

reset_parameters(*self*)

forward(*self*, *x*, *edge_index*)

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

Bases: *cogdl.models.BaseModel*

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

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

reset_parameters(*self*)

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.fastgcn

Module Contents

Classes

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

class cogdl.models.nn.fastgcn.**GraphConvolution**(*in_features*, *out_features*, *bias=True*)

Bases: torch.nn.Module

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

reset_parameters(*self*)

forward(*self*, *input*, *adj*)

__repr__(*self*)

class cogdl.models.nn.fastgcn.**FastGCN**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*, *sample_size*)

Bases: *cogdl.models.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*cls*, *args*)

Build a new model instance.

set_adj(*self*, *edge_index*, *num_nodes*)

_sample_one_layer(*self*, *sampled*, *sample_size*)

_generate_adj(*self*, *sample1*, *sample2*)

sampling(*self*, *x*, *v*)

forward(*self*, *x*, *adj*)

cogdl.models.nn.gat

Module Contents

Classes

SpecialSpmmFunction	Special function for only sparse region backpropataion layer.
SpecialSpmm	
SpGraphAttentionLayer	Sparse version GAT layer, similar to https://arxiv.org/abs/1710.10903
PetarVSpGAT	The GAT model from the `"Graph Attention Networks"

class cogdl.models.nn.gat.**SpecialSpmmFunction**
Bases: torch.autograd.Function

Special function for only sparse region backpropataion layer.

static forward(*ctx*, *indices*, *values*, *shape*, *b*)

static backward(*ctx*, *grad_output*)

class cogdl.models.nn.gat.**SpecialSpmm**
Bases: torch.nn.Module

forward(*self*, *indices*, *values*, *shape*, *b*)

class cogdl.models.nn.gat.**SpGraphAttentionLayer**(*in_features*, *out_features*, *dropout*, *alpha*, *concat=True*)
Bases: torch.nn.Module

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

forward(*self*, *input*, *edge*)

__repr__(*self*)

class cogdl.models.nn.gat.**PetarVSpGAT**(*nfeat*, *nhid*, *nclass*, *dropout*, *alpha*, *nheads*)
Bases: *cogdl.models.BaseModel*

The GAT model from the "Graph Attention Networks" paper

Args: 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(*cls*, *args*)
Build a new model instance.

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.gcn

Module Contents

Classes

GraphConvolution	Simple GCN layer, similar to https://arxiv.org/abs/1609.02907
TKipfGCN	The GCN model from the `"Semi-Supervised Classification with Graph Convolutional Networks"

class cogdl.models.nn.gcn.**GraphConvolution**(*in_features*, *out_features*, *bias=True*)

Bases: torch.nn.Module

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

reset_parameters(*self*)

forward(*self*, *input*, *edge_index*, *edge_attr=None*)

__repr__(*self*)

class cogdl.models.nn.gcn.**TKipfGCN**(*nfeat*, *nhid*, *nclass*, *dropout*)

Bases: *cogdl.models.BaseModel*

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

Args: 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.

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*cls*, *args*)

Build a new model instance.

forward(*self*, *x*, *adj*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.gcnii

Module Contents

Classes

GCNIILayer
GCNII

class cogdl.models.nn.gcnii.**GCNIILayer**(*n_channels*, *alpha=0.1*, *beta=1*, *residual=False*)

Bases: torch.nn.Module

reset_parameters(*self*)

forward(*self*, *x*, *edge_index*, *edge_attr*, *init_x*)

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*)

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*, *edge_attr=None*)

loss(*self*, *data*)

predict(*self*, *data*)

get_optimizer(*self*, *args*)

cogdl.models.nn.graphsage

Module Contents

Classes

GraphSAGELayer	
Graphsage	

Functions

sage_sampler(adjlist, edge_index, num_sample)	

cogdl.models.nn.graphsage.**sage_sampler**(*adjlist*, *edge_index*, *num_sample*)

class cogdl.models.nn.graphsage.**GraphSAGELayer**(*in_feats*, *out_feats*)

Bases: `torch.nn.Module`

forward(*self*, *x*, *edge_index*)

class cogdl.models.nn.graphsage.**Graphsage**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *sample_size*, *dropout*)

Bases: *cogdl.models.BaseModel*

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

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

sampling(*self*, *edge_index*, *num_sample*)

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.mixhop

Module Contents

Classes

MixHop

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

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.mlp

Module Contents

Classes

MLP

class cogdl.models.nn.mlp.**MLP**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*)

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.mvgrl

Module Contents

Classes

Discriminator	
Model	
MVGRL	

Functions

preprocess_features(features)	Row-normalize feature matrix and convert to tuple representation
normalize_adj(adj)	Symmetrically normalize adjacency matrix.
sparse_mx_to_torch_sparse_tensor(sparse_mx)	Convert a scipy sparse matrix to a torch sparse tensor.
compute_ppr(graph: networkx.Graph, alpha=0.2, self_loop=True)	

class cogdl.models.nn.mvgrl.**Discriminator**(*n_h*)
Bases: torch.nn.Module

weights_init(*self*, *m*)

forward(*self*, *c1*, *c2*, *h1*, *h2*, *h3*, *h4*, *s_bias1=None*, *s_bias2=None*)

class cogdl.models.nn.mvgrl.**Model**(*n_in*, *n_h*)
Bases: torch.nn.Module

forward(*self*, *seq1*, *seq2*, *adj*, *diff*, *sparse*, *msk*, *samp_bias1*, *samp_bias2*)

embed(*self*, *seq*, *adj*, *diff*, *sparse*, *msk*)

cogdl.models.nn.mvgrl.**preprocess_features**(*features*)
Row-normalize feature matrix and convert to tuple representation

cogdl.models.nn.mvgrl.**normalize_adj**(*adj*)
Symmetrically normalize adjacency matrix.

cogdl.models.nn.mvgrl.**sparse_mx_to_torch_sparse_tensor**(*sparse_mx*)
Convert a scipy sparse matrix to a torch sparse tensor.

cogdl.models.nn.mvgrl.**compute_ppr**(*graph: networkx.Graph*, *alpha=0.2*, *self_loop=True*)

class cogdl.models.nn.mvgrl.**MVGRL**(*nfeat*, *nhid*, *nclass*, *max_epochs*)
Bases: *cogdl.models.BaseModel*

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

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

train (*self*, *data*, *dataset_name*)

cogdl.models.nn.patchy_san

Module Contents

Classes

PatchySAN	The Patchy-SAN model from the `"Learning Convolutional Neural Networks for Graphs"

Functions

assemble_neighbor(G, node, num_neighbor, sorted_nodes)	assemble neighbors for node with BFS strategy
cmp(s1, s2)	
one_dim_wl(graph_list, init_labels, iteration=5)	1-dimension Wl method used for node normalization for all the subgraphs
node_selection_with_1d_wl(G, features, num_channel, num_sample, num_neighbor, stride)	construct features for cnn
get_single_feature(data, num_features, num_classes, num_sample, num_neighbor, stride=1)	construct features

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

Bases: *cogdl.models.BaseModel*

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

Args: 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.

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

classmethod split_dataset(*self*, *dataset*, *args*)

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

forward(*self*, *batch*)

cogdl.models.nn.patchy_san.**assemble_neighbor**(*G*, *node*, *num_neighbor*, *sorted_nodes*)
assemble neighbors for node with BFS strategy

cogdl.models.nn.patchy_san.**cmp**(*s1*, *s2*)

cogdl.models.nn.patchy_san.**one_dim_wl**(*graph_list*, *init_labels*, *iteration=5*)
1-dimension Wl method used for node normalization for all the subgraphs

cogdl.models.nn.patchy_san.**node_selection_with_1d_wl**(*G*, *features*, *num_channel*, *num_sample*, *num_neighbor*, *stride*)

construct features for cnn

cogdl.models.nn.patchy_san.**get_single_feature**(*data*, *num_features*, *num_classes*, *num_sample*, *num_neighbor*, *stride=1*)

construct features

cogdl.models.nn.pyg_cheb

Module Contents

Classes

Chebyshev

class cogdl.models.nn.pyg_cheb.**Chebyshev**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*, *filter_size*)

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_deepergcn

Module Contents

Classes

GENConv
DeepGCNLayer
DeeperGCN

class cogdl.models.nn.pyg_deepergcn.**GENConv**(*in_feat*, *out_feat*, *aggr='softmax_sg'*, *beta=1.0*, *p=1.0*, *learn_beta=False*, *learn_p=False*, *use_msg_norm=False*, *learn_msg_scale=True*)

Bases: torch.nn.Module

message_norm(*self*, *x*, *msg*)

forward(*self*, *x*, *edge_index*, *edge_attr=None*)

class cogdl.models.nn.pyg_deepergcn.**DeepGCNLayer**(*in_feat*, *out_feat*, *conv*, *connection='res'*, *activation='relu'*, *dropout=0.0*, *checkpoint_grad=False*)

Bases: `torch.nn.Module`

forward(*self*, *x*, *edge_index*)

class cogdl.models.nn.pyg_deepergcn.**DeeperGCN**(*in_feat*, *hidden_size*, *out_feat*, *num_layers*, *connection='res+'*, *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*)

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*, *edge_attr=None*)

loss(*self*, *x*, *edge_index*, *y*, *x_mask*)

predict(*self*, *x*, *edge_index*)

static get_trainer(*taskType: Any*, *args*)

cogdl.models.nn.pyg_dgcnn

Module Contents

Classes

DGCNN	EdgeConv and DynamicGraph in paper `"Dynamic Graph CNN for Learning on

class cogdl.models.nn.pyg_dgcnn.**DGCNN**(*in_feats*, *hidden_dim*, *out_feats*, *k=20*, *dropout=0.5*)

Bases: *cogdl.models.BaseModel*

EdgeConv and DynamicGraph in paper *"Dynamic Graph CNN for Learning on Point Clouds" <https://arxiv.org/pdf/1801.07829.pdf>__* .

in_feats [int] Size of each input sample.

out_feats [int] Size of each output sample.

hidden_dim [int] Dimension of hidden layer embedding.

k [int] Number of neareast neighbors.

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

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

classmethod split_dataset(*cls*, *dataset*, *args*)

forward(*self*, *batch*)

cogdl.models.nn.pyg_diffpool

Module Contents

Classes

EntropyLoss	
LinkPredLoss	
GraphSAGE	GraphSAGE from "Inductive Representation Learning on Large Graphs".
BatchedGraphSAGE	GraphSAGE with mini-batch
BatchedDiffPoolLayer	DIFFPOOL from paper `"Hierarchical Graph Representation Learning
BatchedDiffPool	DIFFPOOL layer with batch forward
DiffPool	DIFFPOOL from paper `Hierarchical Graph Representation Learning

Functions

toBatchedGraph(batch_adj, batch_feat, node_per_pool_graph)	

class cogdl.models.nn.pyg_diffpool.**EntropyLoss**
Bases: torch.nn.Module

forward(*self*, *adj*, *anext*, *s_l*)

class cogdl.models.nn.pyg_diffpool.**LinkPredLoss**
Bases: torch.nn.Module

forward(*self*, *adj*, *anext*, *s_l*)

class cogdl.models.nn.pyg_diffpool.**GraphSAGE**(*in_feats*, *hidden_dim*, *out_feats*, *num_layers*, *dropout=0.5*, *normalize=False*, *concat=False*, *use_bn=False*)
Bases: torch.nn.Module

GraphSAGE from "Inductive Representation Learning on Large Graphs".

..math:: h^{i+1}_{mathcal{N}(v)}=AGGREGATE_{k}(h_{u}^{k}) h^{k+1}_{v} = sigma(mathbf{W}^{k}·CONCAT(h_{v}^{k}, h_{mathcal{N}(v)}))

Args: in_feats (int) : Size of each input sample. hidden_dim (int) : Size of hidden layer dimension. out_feats (int) : Size of each output sample. num_layers (int) : Number of GraphSAGE Layers. dropout (float,

optional) : Size of dropout, default: `0.5`. normalize (bool, optional) : Normalze features after each layer if True, default: `True`.

forward(*self*, *x*, *edge_index*, *edge_weight=None*)

class cogdl.models.nn.pyg_diffpool.**BatchedGraphSAGE**(*in_feats*, *out_feats*, *use_bn=True*, *self_loop=True*)

Bases: `torch.nn.Module`

GraphSAGE with mini-batch

Args: in_feats (int) : Size of each input sample. out_feats (int) : Size of each output sample. use_bn (bool) : Apply batch normalization if True, default: `True`. self_loop (bool) : Add self loop if True, default: `True`.

forward(*self*, *x*, *adj*)

class cogdl.models.nn.pyg_diffpool.**BatchedDiffPoolLayer**(*in_feats*, *out_feats*, *assign_dim*, *batch_size*, *dropout=0.5*, *link_pred_loss=True*, *entropy_loss=True*)

Bases: `torch.nn.Module`

DIFFPOOL from paper "Hierarchical Graph Representation Learning with Differentiable Pooling".

$$X^{(l+1)} = S^{l)T} Z^{(l)} A^{(l+1)} = S^{(l)T} A^{(l)} S^{(l)} Z^{(l)} = GNN_{l,embed}(A^{(l)}, X^{(l)}) S^{(l)} = softmax(GNN_{l,pool}(A^{(l)}, X^{(l)}))$$

in_feats [int] Size of each input sample.

out_feats [int] Size of each output sample.

assign_dim [int] Size of next adjacency matrix.

batch_size [int] Size of each mini-batch.

dropout [float, optional] Size of dropout, default: `0.5`.

link_pred_loss [bool, optional] Use link prediction loss if True, default: `True`.

forward(*self*, *x*, *edge_index*, *batch*, *edge_weight=None*)

get_loss(*self*)

class cogdl.models.nn.pyg_diffpool.**BatchedDiffPool**(*in_feats*, *next_size*, *emb_size*, *use_bn=True*, *self_loop=True*, *use_link_loss=False*, *use_entropy=True*)

Bases: `torch.nn.Module`

DIFFPOOL layer with batch forward

in_feats [int] Size of each input sample.

next_size [int] Size of next adjacency matrix.

emb_size [int] Dimension of next node feature matrix.

use_bn [bool, optional] Apply batch normalization if True, default: `True`.

self_loop [bool, optional] Add self loop if True, default: `True`.

use_link_loss [bool, optional] Use link prediction loss if True, default: `True`.

use_entropy [bool, optioinal] Use entropy prediction loss if True, default: `True`.

forward(*self*, *x*, *adj*)

get_loss(*self*)

cogdl.models.nn.pyg_diffpool.**toBatchedGraph**(*batch_adj*, *batch_feat*, *node_per_pool_graph*)

class cogdl.models.nn.pyg_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.BaseModel*

DIFFPOOL from paper Hierarchical Graph Representation Learning with Differentiable Pooling.

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.

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

classmethod split_dataset(*cls*, *dataset*, *args*)

reset_parameters(*self*)

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

forward(*self*, *batch*)

loss(*self*, *prediction*, *label*)

cogdl.models.nn.pyg_drgat

Module Contents

Classes

DrGAT

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

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_drgcn

Module Contents

Classes

DrGCN

class cogdl.models.nn.pyg_drgcn.**DrGCN**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*)

Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_gat

Module Contents

Classes

GAT

class cogdl.models.nn.pyg_gat.**GAT**(*num_features*, *num_classes*, *hidden_size*, *num_heads*, *dropout*)

Bases: *cogdl.models.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_gcn

Module Contents

Classes

GCN

class cogdl.models.nn.pyg_gcn.**GCN**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*)
Bases: *cogdl.models.BaseModel*

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

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

get_trainer(*self*, *task*, *args*)

forward(*self*, *x*, *edge_index*, *weight=None*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_gcnmix

Module Contents

Classes

GCNConv
BaseGNNMix
GCNMix

Functions

mix_hidden_state(feat, target, train_index, alpha)
sharpen(prob, temperature)
get_one_hot_label(labels, index)
get_current_consistency_weight(final_consistency_weight, rampup_starts, rampup_ends, epoch)

cogdl.models.nn.pyg_gcnmix.**mix_hidden_state**(*feat*, *target*, *train_index*, *alpha*)

cogdl.models.nn.pyg_gcnmix.**sharpen**(*prob*, *temperature*)

cogdl.models.nn.pyg_gcnmix.**get_one_hot_label**(*labels*, *index*)

cogdl.models.nn.pyg_gcnmix.**get_current_consistency_weight**(*final_consistency_weight*, *rampup_starts*, *rampup_ends*, *epoch*)

class cogdl.models.nn.pyg_gcnmix.**GCNConv**(*in_feats*, *out_feats*)

Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr=None*)

forward_aux(*self*, *x*)

class cogdl.models.nn.pyg_gcnmix.**BaseGNNMix**(*in_feat*, *hidden_size*, *num_classes*, *k*, *temperature*, *alpha*, *dropout*)

Bases: *cogdl.models.BaseModel*

forward(*self*, *x*, *edge_index*)

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

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

update_soft(*self*, *data*, *labels*, *train_index*)

loss(*self*, *data*, *opt*)

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

class cogdl.models.nn.pyg_gcnmix.**GCNMix**(*in_feat*, *hidden_size*, *num_classes*, *k*, *temperature*, *alpha*, *rampup_starts*, *rampup_ends*, *final_consistency_weight*, *ema_decay*, *dropout*)

Bases: *cogdl.models.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*cls*, *args*)

Build a new model instance.

forward(*self*, *x*, *edge_index*)

forward_ema(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_gin

Module Contents

Classes

GINLayer	Graph Isomorphism Network layer from paper `"How Powerful are Graph
GINMLP	Multilayer perception with batch normalization
GIN	Graph Isomorphism Network from paper `"How Powerful are Graph

class cogdl.models.nn.pyg_gin.**GINLayer**(*apply_func=None*, *eps=0*, *train_eps=True*)

Bases: torch.nn.Module

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

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

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(*self*, *x*, *edge_index*, *edge_weight=None*)

class cogdl.models.nn.pyg_gin.**GINMLP**(*in_feats*, *out_feats*, *hidden_dim*, *num_layers*, *use_bn=True*, *activation=None*)

Bases: torch.nn.Module

Multilayer perception with batch normalization

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

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(*self*, *x*)

class cogdl.models.nn.pyg_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.BaseModel*

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

Args:

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(*cls*, *args*)
Build a new model instance.

classmethod split_dataset(*cls*, *dataset*, *args*)

forward(*self*, *batch*)

loss(*self*, *output*, *label=None*)

cogdl.models.nn.pyg_gpt_gnn

Module Contents

Classes

GPT_GNN	Helper class that provides a standard way to create an ABC using

class cogdl.models.nn.pyg_gpt_gnn.**GPT_GNN**
Bases: *cogdl.models.supervised_model.SupervisedHomogeneousNodeClassificationModel*, *cogdl.models.supervised_model.SupervisedHeterogeneousNodeClassificationModel*

Helper class that provides a standard way to create an ABC using inheritance.

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

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

loss(*self*, *data: Any*) → Any

predict(*self*, *data: Any*) → Any

evaluate(*self*, *data: Any*, *nodes: Any*, *targets: Any*) → Any

static get_trainer(*taskType: Any*, *args*) → Optional[Type[Union[GPT_GNNHomogeneousTrainer, GPT_GNNHeterogeneousTrainer]]]

cogdl.models.nn.pyg_grand

Module Contents

Classes

MLPLayer
Grand

class cogdl.models.nn.pyg_grand.**MLPLayer**(*in_features*, *out_features*, *bias=True*)

Bases: torch.nn.Module

reset_parameters(*self*)

forward(*self*, *x*)

__repr__(*self*)

class cogdl.models.nn.pyg_grand.**Grand**(*nfeat*, *nhid*, *nclass*, *input_droprate*, *hidden_droprate*, *use_bn*, *dropnode_rate*, *tem*, *lam*, *order*, *sample*, *alpha*)

Bases: *cogdl.models.BaseModel*

static add_args(*parser*)

Add model-specific arguments to the parser.

classmethod build_model_from_args(*cls*, *args*)

Build a new model instance.

dropNode(*self*, *x*)

normalize_adj(*self*, *edge_index*, *edge_weight*, *num_nodes*)

rand_prop(*self*, *x*, *edge_index*, *edge_weight*)

consis_loss(*self*, *logps*, *train_mask*)

normalize_x(*self*, *x*)

forward(*self*, *x*, *edge_index*)

adj = torch.sparse_coo_tensor(edge_index, torch.ones(edge_index.shape[1]).float(), (x.shape[0], x.shape[0]),

).to(x.device)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_gtn

Module Contents

Classes

GTConv
GTLayer
GTN

class cogdl.models.nn.pyg_gtn.**GTConv**(*in_channels*, *out_channels*, *num_nodes*)
Bases: torch.nn.Module

reset_parameters(*self*)

forward(*self*, *A*)

class cogdl.models.nn.pyg_gtn.**GTLayer**(*in_channels*, *out_channels*, *num_nodes*, *first=True*)
Bases: torch.nn.Module

forward(*self*, *A*, *H_=None*)

class cogdl.models.nn.pyg_gtn.**GTN**(*num_edge*, *num_channels*, *w_in*, *w_out*, *num_class*, *num_nodes*, *num_layers*)
Bases: *cogdl.models.BaseModel*

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

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

normalization(*self*, *H*)

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

forward(*self*, *A*, *X*, *target_x*, *target*)

loss(*self*, *data*)

evaluate(*self*, *data*, *nodes*, *targets*)

cogdl.models.nn.pyg_han

Module Contents

Classes

AttentionLayer
HANLayer

continues on next page

Table 102 – continued from previous page

HAN	

class cogdl.models.nn.pyg_han.**AttentionLayer**(*num_features*)
Bases: torch.nn.Module

forward(*self*, *x*)

class cogdl.models.nn.pyg_han.**HANLayer**(*num_edge*, *w_in*, *w_out*)
Bases: torch.nn.Module

forward(*self*, *x*, *adj*)

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

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

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

forward(*self*, *A*, *X*, *target_x*, *target*)

loss(*self*, *data*)

evaluate(*self*, *data*, *nodes*, *targets*)

cogdl.models.nn.pyg_infograph

Module Contents

Classes

SUPEncoder	Encoder used in supervised model with Set2set in paper `"Order Matters: Sequence to sequence for sets"
Encoder	Encoder stacked with GIN layers
FF	Residual MLP layers.
InfoGraph	Implimentation of Infograph in paper `"InfoGraph: Unsupervised and Semi-supervised Graph-Level Representation

class cogdl.models.nn.pyg_infograph.**SUPEncoder**(*num_features*, *dim*, *num_layers=1*)
Bases: torch.nn.Module

Encoder used in supervised model with Set2set in paper *"Order Matters: Sequence to sequence for sets" <https://arxiv.org/abs/1511.06391>* and NNConv in paper *"Dynamic Edge-Conditioned Filters in Convolutional Neural Networks on Graphs" <https://arxiv.org/abs/1704.02901>*

forward(*self*, *x*, *edge_index*, *batch*, *edge_attr*)

class cogdl.models.nn.pyg_infograph.**Encoder**(*in_feats*, *hidden_dim*, *num_layers=3*, *num_mlp_layers=2*, *pooling='sum'*)
Bases: torch.nn.Module

Encoder stacked with GIN layers

in_feats [int] Size of each input sample.

hidden_feats [int] Size of output embedding.

num_layers [int, optional] Number of GIN layers, default: `3`.

num_mlp_layers [int, optional] Number of MLP layers for each GIN layer, default: `2`.

pooling [str, optional] Aggragation type, default : `sum`.

forward(*self*, *x*, *edge_index*, *batch*, **args*)

class cogdl.models.nn.pyg_infograph.**FF**(*in_feats*, *out_feats*)

Bases: `torch.nn.Module`

Residual MLP layers.

..math:: out = mathbf{MLP}(x) + mathbf{Linear}(x)

in_feats [int] Size of each input sample

out_feats [int] Size of each output sample

forward(*self*, *x*)

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

Bases: *cogdl.models.BaseModel*

**Implimentation 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(*cls*, *args*)
Build a new model instance.

classmethod split_dataset(*cls*, *dataset*, *args*)

reset_parameters(*self*)

forward(*self*, *batch*)

sup_forward(*self*, *x*, *edge_index=None*, *batch=None*, *label=None*, *edge_attr=None*)

unsup_forward(*self*, *x*, *edge_index=None*, *batch=None*)

sup_loss(*self*, *prediction*, *label=None*)

unsup_loss(*self*, *x*, *edge_index=None*, *batch=None*)

unsup_sup_loss(*self*, *x*, *edge_index*, *batch*)

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

cogdl.models.nn.pyg_infomax

Module Contents

Classes

Encoder	
Infomax	

Functions

corruption(x, edge_index)	

class cogdl.models.nn.pyg_infomax.**Encoder**(*in_channels*, *hidden_channels*)
Bases: torch.nn.Module

forward(*self*, *x*, *edge_index*)

cogdl.models.nn.pyg_infomax.**corruption**(*x*, *edge_index*)

class cogdl.models.nn.pyg_infomax.**Infomax**(*num_features*, *num_classes*, *hidden_size*)
Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_sortpool

Module Contents

Classes

SortPool	Implimentation of sortpooling in paper `"An End-to-End Deep Learning

Functions

scatter_sum(src, index, dim, dim_size)	
spare2dense_batch(x, batch=None, fill_value=0)	

cogdl.models.nn.pyg_sortpool.**scatter_sum**(*src*, *index*, *dim*, *dim_size*)

cogdl.models.nn.pyg_sortpool.**spare2dense_batch**(*x*, *batch=None*, *fill_value=0*)

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

Bases: *cogdl.models.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>__.*

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(*cls*, *args*)
Build a new model instance.

classmethod split_dataset(*cls*, *dataset*, *args*)

forward(*self*, *batch*)

cogdl.models.nn.pyg_srgcn

Module Contents

Classes

NodeAdaptiveEncoder	
SrgcnHead	

continues on next page

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SrgcnSoftmaxHead
SRGCN

class cogdl.models.nn.pyg_srgcn.**NodeAdaptiveEncoder**(*num_features*, *dropout=0.5*)
Bases: cogdl.layers.srgcn_module.nn.Module

forward(*self*, *x*)

class cogdl.models.nn.pyg_srgcn.**SrgcnHead**(*num_features*, *out_feats*, *attention*, *activation*, *normalization*, *nhop*, *subheads=2*, *dropout=0.5*, *node_dropout=0.5*, *alpha=0.2*, *concat=True*)
Bases: cogdl.layers.srgcn_module.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*)

class cogdl.models.nn.pyg_srgcn.**SrgcnSoftmaxHead**(*num_features*, *out_feats*, *attention*, *activation*, *nhop*, *normalization*, *dropout=0.5*, *node_dropout=0.5*, *alpha=0.2*)
Bases: cogdl.layers.srgcn_module.nn.Module

forward(*self*, *x*, *edge_index*, *edge_attr*)

class cogdl.models.nn.pyg_srgcn.**SRGCN**(*num_features*, *hidden_size*, *num_classes*, *attention*, *activation*, *nhop*, *normalization*, *dropout*, *node_dropout*, *alpha*, *nhead*, *subheads*)
Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *batch*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_stpgnn

Module Contents

Classes

stpgnn

class cogdl.models.nn.pyg_stpgnn.**stpgnn**(*args*)
Bases: *cogdl.models.BaseModel*

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

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

cogdl.models.nn.pyg_unet

Module Contents

Classes

UNet

class cogdl.models.nn.pyg_unet.**UNet**(*num_features*, *num_classes*, *hidden_size*, *num_layers*, *dropout*, *num_nodes*)
Bases: *cogdl.models.BaseModel*

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

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

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

predict(*self*, *data*)

cogdl.models.nn.pyg_unsup_graphsage

Module Contents

Classes

SAGE
Graphsage

class cogdl.models.nn.pyg_unsup_graphsage.**SAGE**(*num_features*, *hidden_size*, *num_layers*, *sample_size*, *dropout*, *walk_length*, *negative_samples*)
Bases: `torch.nn.Module`

sampling(*self*, *edge_index*, *num_sample*)

forward(*self*, *x*, *edge_index*)

loss(*self*, *data*)

embed(*self*, *data*)

class cogdl.models.nn.pyg_unsup_graphsage.**Graphsage**(*num_features*, *hidden_size*, *num_classes*, *num_layers*, *sample_size*, *dropout*, *walk_length*, *negative_samples*, *lr*, *epochs*, *patience*)

Bases: *cogdl.models.BaseModel*

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

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

train(*self*, *data*)

cogdl.models.nn.rgcn

Module Contents

Classes

RGCNLayer
RGCN
LinkPredictRGCN

class cogdl.models.nn.rgcn.**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.Module`

reset_parameters(*self*)

forward(*self*, *x*, *edge_index*, *edge_type*)

basis_forward(*self*, *x*, *edge_index*, *edge_type*)

bdd_forward(*self*, *x*, *edge_index*, *edge_type*)

class cogdl.models.nn.rgcn.**RGCN**(*in_feats*, *out_feats*, *num_layers*, *num_rels*, *regularizer='basis'*, *num_bases=None*, *self_loop=True*, *dropout=0.0*, *self_dropout=0.0*)

Bases: `torch.nn.Module`

forward(*self*, *x*, *edge_index*, *edge_type*)

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.layers.link_prediction_module.GNNLinkPredict*, *cogdl.models.BaseModel*

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

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

forward(*self*, *edge_index*, *edge_type*)

loss(*self*, *data*, *split='train'*)

predict(*self*, *edge_index*, *edge_type*)

Submodules

cogdl.models.base_model

Module Contents

Classes

BaseModel

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

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

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

_forward_unimplemented(*self*, **input: Any*) → None

static get_trainer(*taskType: Any*, *args: Any*) → Optional[Type[BaseTrainer]]

cogdl.models.supervised_model

Module Contents

Classes

SupervisedModel	Helper class that provides a standard way to create an ABC using
SupervisedHeterogeneousNodeClassificationModel	Helper class that provides a standard way to create an ABC using
SupervisedHomogeneousNodeClassificationModel	Helper class that provides a standard way to create an ABC using

class cogdl.models.supervised_model.**SupervisedModel**
Bases: *cogdl.models.BaseModel*, abc.ABC

Helper class that provides a standard way to create an ABC using inheritance.

abstract loss(*self*, *data: Any*) → Any

class cogdl.models.supervised_model.**SupervisedHeterogeneousNodeClassificationModel**
Bases: *cogdl.models.BaseModel*, abc.ABC

Helper class that provides a standard way to create an ABC using inheritance.

abstract loss(*self*, *data: Any*) → Any

evaluate(*self*, *data: Any*, *nodes: Any*, *targets: Any*) → Any

static get_trainer(*taskType: Any*, *args: Any*) → Optional[Type[SupervisedHeterogeneousNodeClassificationTrainer]]

class cogdl.models.supervised_model.**SupervisedHomogeneousNodeClassificationModel**
Bases: *cogdl.models.BaseModel*, abc.ABC

Helper class that provides a standard way to create an ABC using inheritance.

abstract loss(*self*, *data: Any*) → Any

abstract predict(*self*, *data: Any*) → Any

static get_trainer(*taskType: Any*, *args: Any*) → Optional[Type[SupervisedHomogeneousNodeClassificationTrainer]]

Package Contents

Classes

BaseModel	

Functions

register_model(name)	New model types can be added to cogdl with the *register_model()*
alias_setup(probs)	Compute utility lists for non-uniform sampling from discrete distributions.
alias_draw(J, q)	Draw sample from a non-uniform discrete distribution using alias sampling.
build_model(args)	

class cogdl.models.**BaseModel**
Bases: torch.nn.Module

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

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

_forward_unimplemented(*self*, **input: Any*) → None

static get_trainer(*taskType: Any*, *args: Any*) → Optional[Type[BaseTrainer]]

cogdl.models.**pyg = False**

cogdl.models.**dgl_import = False**

cogdl.models.**MODEL_REGISTRY**

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):
    (...)
```

Args: name (str): the name of the model

cogdl.models.**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.models.**alias_draw**(*J*, *q*)

Draw sample from a non-uniform discrete distribution using alias sampling.

cogdl.models.**model_name**

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

cogdl.tasks

Submodules

cogdl.tasks.base_task

Module Contents

Classes

BaseTask

class cogdl.tasks.base_task.**BaseTask**(*args*)

Bases: object

static add_args(*parser*)

Add task-specific arguments to the parser.

abstract train(*self*, *num_epoch*)

cogdl.tasks.graph_classification

Module Contents

Classes

GraphClassification	Superiviced graph classification task.

Functions

node_degree_as_feature(data)	Set each node feature as one-hot encoding of degree
uniform_node_feature(data)	Set each node feature to the same

cogdl.tasks.graph_classification.**node_degree_as_feature**(*data*)
Set each node feature as one-hot encoding of degree :param data: a list of class Data :return: a list of class Data

cogdl.tasks.graph_classification.**uniform_node_feature**(*data*)
Set each node feature to the same

class cogdl.tasks.graph_classification.**GraphClassification**(*args*, *dataset=None*, *model=None*)

Bases: *cogdl.tasks.BaseTask*

Superiviced graph classification task.

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

train(*self*)

_train(*self*)

_train_step(*self*)

_test_step(*self*, *split='val'*)

_kfold_train(*self*)

generate_data(*self*, *dataset*, *args*)

cogdl.tasks.heterogeneous_node_classification

Module Contents

Classes

HeterogeneousNodeClassification	Heterogeneous Node classification task.

class cogdl.tasks.heterogeneous_node_classification.**HeterogeneousNodeClassification**(*args*, *dataset=N*, *model=N*

Bases: *cogdl.tasks.BaseTask*

Heterogeneous Node classification task.

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

train(*self*)

_train_step(*self*)

_test_step(*self*, *split='val'*)

cogdl.tasks.link_prediction

Module Contents

Classes

HomoLinkPrediction	
TripleLinkPrediction	Training process borrowed from *KnowledgeGraphEmbedding<https://github.com/DeepGraphLearning/KnowledgeGraphEmbedding*
KGLinkPrediction	
LinkPrediction	

Functions

save_model(model, optimizer, save_variable_list, args)	Save the parameters of the model and the optimizer,
set_logger(args)	Write logs to checkpoint and console
log_metrics(mode, step, metrics)	Print the evaluation logs
divide_data(input_list, division_rate)	
randomly_choose_false_edges(nodes, true_edges, num)	
gen_node_pairs(train_data, test_data, negative_ratio=5)	
get_score(embs, node1, node2)	
evaluate(embs, true_edges, false_edges)	
select_task(model_name=None, model=None)	

cogdl.tasks.link_prediction.**save_model**(*model*, *optimizer*, *save_variable_list*, *args*)
Save the parameters of the model and the optimizer, as well as some other variables such as step and learning_rate

cogdl.tasks.link_prediction.**set_logger**(*args*)

Write logs to checkpoint and console

cogdl.tasks.link_prediction.**log_metrics**(*mode*, *step*, *metrics*)
Print the evaluation logs

cogdl.tasks.link_prediction.**divide_data**(*input_list*, *division_rate*)

cogdl.tasks.link_prediction.**randomly_choose_false_edges**(*nodes*, *true_edges*, *num*)

cogdl.tasks.link_prediction.**gen_node_pairs**(*train_data*, *test_data*, *negative_ratio=5*)

cogdl.tasks.link_prediction.**get_score**(*embs*, *node1*, *node2*)

cogdl.tasks.link_prediction.**evaluate**(*embs*, *true_edges*, *false_edges*)

cogdl.tasks.link_prediction.**select_task**(*model_name=None*, *model=None*)

class cogdl.tasks.link_prediction.**HomoLinkPrediction**(*args*, *dataset=None*, *model=None*)
Bases: torch.nn.Module

train(*self*)

class cogdl.tasks.link_prediction.**TripleLinkPrediction**(*args*, *dataset=None*, *model=None*)
Bases: torch.nn.Module

Training process borrowed from *KnowledgeGraphEmbedding<https://github.com/DeepGraphLearning/KnowledgeGraphEmbeda*

train(*self*)

class cogdl.tasks.link_prediction.**KGLinkPrediction**(*args*, *dataset=None*, *model=None*)
Bases: torch.nn.Module

train(*self*)

_train_step(*self*, *split='train'*)

_test_step(*self*, *split='val'*)

class cogdl.tasks.link_prediction.**LinkPrediction**(*args*, *dataset=None*, *model=None*)
Bases: *cogdl.tasks.BaseTask*

static add_args(*parser*)

train(*self*)

cogdl.tasks.multiplex_link_prediction

Module Contents

Classes

MultiplexLinkPrediction

Functions

get_score(embs, node1, node2)	
evaluate(embs, true_edges, false_edges)	

cogdl.tasks.multiplex_link_prediction.**get_score**(*embs*, *node1*, *node2*)

cogdl.tasks.multiplex_link_prediction.**evaluate**(*embs*, *true_edges*, *false_edges*)

class cogdl.tasks.multiplex_link_prediction.**MultiplexLinkPrediction**(*args*, *dataset=None*, *model=None*)

Bases: *cogdl.tasks.BaseTask*

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

train(*self*)

cogdl.tasks.multiplex_node_classification

Module Contents

Classes

MultiplexNodeClassification	Node classification task.

class cogdl.tasks.multiplex_node_classification.**MultiplexNodeClassification**(*args*, *dataset=None*, *model=None*)

Bases: *cogdl.tasks.BaseTask*

Node classification task.

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

train(*self*)

cogdl.tasks.node_classification

Module Contents

Classes

NodeClassification	Node classification task.

class cogdl.tasks.node_classification.**NodeClassification**(*args*, *dataset=None*, *model: Optional[SupervisedHomogeneousNodeClassificatio = None*)

Bases: *cogdl.tasks.BaseTask*

Node classification task.

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

train(*self*)

_train_step(*self*)

_test_step(*self*, *split='val'*, *logits=None*)

cogdl.tasks.node_classification_sampling

Module Contents

Classes

NodeClassificationSampling	Node classification task with sampling.

Functions

get_batches(train_nodes, train_labels, batch_size=64, shuffle=True)	

cogdl.tasks.node_classification_sampling.**get_batches**(*train_nodes*, *train_labels*, *batch_size=64*, *shuffle=True*)

class cogdl.tasks.node_classification_sampling.**NodeClassificationSampling**(*args*, *dataset=None*, *model=None*)

Bases: *cogdl.tasks.BaseTask*

Node classification task with sampling.

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

train(*self*)

_train_step(*self*)

_test_step(*self*, *split='val'*)

cogdl.tasks.pretrain

Module Contents

Classes

PretrainTask	

class cogdl.tasks.pretrain.**PretrainTask**(*args*)

Bases: *cogdl.tasks.BaseTask*

static add_args(*parser*)

Add task-specific arguments to the parser.

train(*self*)

cogdl.tasks.unsupervised_graph_classification

Module Contents

Classes

UnsupervisedGraphClassification	Unsupervised graph classification

class cogdl.tasks.unsupervised_graph_classification.**UnsupervisedGraphClassification**(*args*, *dataset=N*, *model=N*

Bases: *cogdl.tasks.BaseTask*

Unsupervised graph classification

static add_args(*parser*)

Add task-specific arguments to the parser.

train(*self*)

save_emb(*self*, *embs*)

_evaluate(*self*, *embeddings*, *labels*)

cogdl.tasks.unsupervised_node_classification

Module Contents

Classes

UnsupervisedNodeClassification	Node classification task.
TopKRanker	

cogdl.tasks.unsupervised_node_classification.**pyg = False**

class cogdl.tasks.unsupervised_node_classification.**UnsupervisedNodeClassification**(*args*, *dataset=Nor*
model=None

Bases: *cogdl.tasks.BaseTask*

Node classification task.

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

enhance_emb(*self*, *G*, *embs*)

save_emb(*self*, *embs*)

train(*self*)

_evaluate(*self*, *features_matrix*, *label_matrix*, *num_shuffle*)

class cogdl.tasks.unsupervised_node_classification.**TopKRanker**
Bases: sklearn.multiclass.OneVsRestClassifier

predict(*self*, *X*, *top_k_list*)

Package Contents

Classes

BaseTask	

Functions

register_task(name)	New task types can be added to cogdl with the *register_task()*
build_task(args, dataset=None, model=None)	

class cogdl.tasks.**BaseTask**(*args*)
Bases: object

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

abstract train(*self*, *num_epoch*)

cogdl.tasks.**TASK_REGISTRY**

cogdl.tasks.**register_task**(*name*)
New task types can be added to cogdl with the *register_task()* function decorator.

For example:

```
@register_task('node_classification')
class NodeClassification(BaseTask):
    (...)
```

Args: name (str): the name of the task

cogdl.tasks.**task_name**

cogdl.tasks.**build_task**(*args*, *dataset=None*, *model=None*)

cogdl.trainers

Submodules

cogdl.trainers.base_trainer

Module Contents

Classes

BaseTrainer	Helper class that provides a standard way to create an ABC using

class cogdl.trainers.base_trainer.**BaseTrainer**

Bases: abc.ABC

Helper class that provides a standard way to create an ABC using inheritance.

abstract classmethod build_trainer_from_args(*cls*, *args*)

Build a new trainer instance.

cogdl.trainers.deepergcn_trainer

Module Contents

Classes

DeeperGCNTrainer	Helper class that provides a standard way to create an ABC using

Functions

random_partition_graph(num_nodes, cluster_number=10)	
generate_subgraphs(edge_index, parts, cluster_number=10, batch_size=1)	

cogdl.trainers.deepergcn_trainer.**random_partition_graph**(*num_nodes*, *cluster_number=10*)

cogdl.trainers.deepergcn_trainer.**generate_subgraphs**(*edge_index*, *parts*, *cluster_number=10*, *batch_size=1*)

class cogdl.trainers.deepergcn_trainer.**DeeperGCNTrainer**(*args*)
Bases: *cogdl.trainers.base_trainer.BaseTrainer*

Helper class that provides a standard way to create an ABC using inheritance.

fit(*self*, *model*, *data*)

test_gpu_volume(*self*)

_train_step(*self*)

_test_step(*self*, *split='val'*)

loss(*self*, *data*)

predict(*self*, *data*)

classmethod build_trainer_from_args(*cls*, *args*)
Build a new trainer instance.

cogdl.trainers.gpt_gnn_trainer

Module Contents

Classes

GPT_GNNHomogeneousTrainer
GPT_GNNHeterogeneousTrainer

Functions

node_classification_sample(args, target_type, seed, nodes, time_range)	sub-graph sampling and label preparation for node classification:
prepare_data(args, graph, target_type, train_target_nodes, valid_target_nodes, pool)	Sampled and prepare training and validation data using multi-process parallization.

cogdl.trainers.gpt_gnn_trainer.**graph_pool**

cogdl.trainers.gpt_gnn_trainer.**node_classification_sample**(*args*, *target_type*, *seed*, *nodes*, *time_range*)
sub-graph sampling and label preparation for node classification: (1) Sample batch_size number of output nodes (papers) and their time.

cogdl.trainers.gpt_gnn_trainer.**prepare_data**(*args*, *graph*, *target_type*, *train_target_nodes*, *valid_target_nodes*, *pool*)
Sampled and prepare training and validation data using multi-process parallization.

class cogdl.trainers.gpt_gnn_trainer.**GPT_GNNHomogeneousTrainer**(*args*)
Bases: *cogdl.trainers.supervised_trainer.SupervisedHomogeneousNodeClassificationTrainer*

fit(*self*, *model:* cogdl.models.supervised_model.SupervisedHeterogeneousNodeClassificationModel, *dataset:* cogdl.data.Dataset) → None

classmethod build_trainer_from_args(*cls*, *args*)

class cogdl.trainers.gpt_gnn_trainer.**GPT_GNNHeterogeneousTrainer**(*model*, *dataset*)

Bases: *cogdl.trainers.supervised_trainer.SupervisedHeterogeneousNodeClassificationTrainer*

fit(*self*) → None

evaluate(*self*, *data: Any*, *nodes: Any*, *targets: Any*) → Any

cogdl.trainers.sampled_trainer

Module Contents

Classes

SampledTrainer	
SAINTTrainer	

class cogdl.trainers.sampled_trainer.**SampledTrainer**

Bases: *cogdl.trainers.supervised_trainer.SupervisedHeterogeneousNodeClassificationTrainer*

abstract fit(*self*, *model:* cogdl.models.supervised_model.SupervisedHeterogeneousNodeClassificationModel, *dataset:* cogdl.data.Dataset)

class cogdl.trainers.sampled_trainer.**SAINTTrainer**(*args*)

Bases: *cogdl.trainers.sampled_trainer.SampledTrainer*

static build_trainer_from_args(*args*)

sampler_from_args(*self*, *args*)

fit(*self*, *model:* cogdl.models.supervised_model.SupervisedHeterogeneousNodeClassificationModel, *dataset:* cogdl.data.Dataset)

_train_step(*self*)

_test_step(*self*, *split='val'*)

cogdl.trainers.supervised_trainer

Module Contents

Classes

SupervisedTrainer	Helper class that provides a standard way to create an ABC using
SupervisedHeterogeneousNodeClassificationTrainer	Helper class that provides a standard way to create an ABC using

continues on next page

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SupervisedHomogeneousNodeClassificationTrainer	Helper class that provides a standard way to create an ABC using

class cogdl.trainers.supervised_trainer.**SupervisedTrainer**
Bases: *cogdl.trainers.base_trainer.BaseTrainer*, abc.ABC

Helper class that provides a standard way to create an ABC using inheritance.

abstract fit(*self*) → None

abstract predict(*self*) → Any

class cogdl.trainers.supervised_trainer.**SupervisedHeterogeneousNodeClassificationTrainer**
Bases: *cogdl.trainers.base_trainer.BaseTrainer*, abc.ABC

Helper class that provides a standard way to create an ABC using inheritance.

abstract fit(*self*, *model:* cogdl.models.supervised_model.SupervisedHeterogeneousNodeClassificationModel, *dataset:* cogdl.data.Dataset) → None

class cogdl.trainers.supervised_trainer.**SupervisedHomogeneousNodeClassificationTrainer**
Bases: *cogdl.trainers.base_trainer.BaseTrainer*, abc.ABC

Helper class that provides a standard way to create an ABC using inheritance.

abstract fit(*self*, *model:* cogdl.models.supervised_model.SupervisedHomogeneousNodeClassificationModel, *dataset:* cogdl.data.Dataset) → None

cogdl.trainers.unsupervised_trainer

Module Contents

Classes

UnsupervisedTrainer	

class cogdl.trainers.unsupervised_trainer.**UnsupervisedTrainer**
Bases: *cogdl.trainers.base_trainer.BaseTrainer*

abstract get_embedding(*self*)

6.1.2 Submodules

cogdl.options

Module Contents

Functions

get_parser()	
add_task_args(parser)	
add_dataset_args(parser)	
add_model_args(parser)	
get_training_parser()	
get_display_data_parser()	
get_download_data_parser()	
parse_args_and_arch(parser, args)	The parser doesn't know about model-specific args, so we parse twice.

cogdl.options.**get_parser**()

cogdl.options.**add_task_args**(*parser*)

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

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

cogdl.options.**get_training_parser**()

cogdl.options.**get_display_data_parser**()

cogdl.options.**get_download_data_parser**()

cogdl.options.**parse_args_and_arch**(*parser*, *args*)
The parser doesn't know about model-specific args, so we parse twice.

cogdl.utils

Module Contents

Classes

ArgClass	

Functions

build_args_from_dict(dic)	
add_self_loops(edge_index, edge_weight=None, fill_value=1, num_nodes=None)	
add_remaining_self_loops(edge_index, edge_weight=None, fill_value=1, num_nodes=None)	

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row_normalization(num_nodes, edge_index, edge_weight=None)	
symmetric_normalization(num_nodes, edge_index, edge_weight=None)	
spmm(indices, values, b)	Args:
spmm_adj(indices, values, shape, b)	
get_degrees(indices, num_nodes=None)	
edge_softmax(indices, values, shape)	Args:
mul_edge_softmax(indices, values, shape)	Args:
remove_self_loops(indices)	
get_activation(act)	
cycle_index(num, shift)	
batch_sum_pooling(x, batch)	
batch_mean_pooling(x, batch)	
tabulate_results(results_dict)	
print_result(results, datasets, model_name)	
set_random_seed(seed)	

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

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

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

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

cogdl.utils.**row_normalization**(*num_nodes*, *edge_index*, *edge_weight=None*)

cogdl.utils.**symmetric_normalization**(*num_nodes*, *edge_index*, *edge_weight=None*)

cogdl.utils.**spmm**(*indices*, *values*, *b*)
Args: indices : Tensor, shape=(2, E) values : Tensor, shape=(E,) shape : tuple(int ,int) b : Tensor, shape=(N,)

cogdl.utils.**spmm_adj**(*indices*, *values*, *shape*, *b*)

cogdl.utils.**get_degrees**(*indices*, *num_nodes=None*)

cogdl.utils.**edge_softmax**(*indices*, *values*, *shape*)

Args: indices: Tensor, shape=(2, E) values: Tensor, shape=(N,) shape: tuple(int, int)

Returns: Softmax values of edge values for nodes

cogdl.utils.**mul_edge_softmax**(*indices*, *values*, *shape*)

Args: indices: Tensor, shape=(2, E) values: Tensor, shape=(E, d) shape: tuple(int, int)

Returns: Softmax values of multi-dimension edge values for nodes

cogdl.utils.**remove_self_loops**(*indices*)

cogdl.utils.**get_activation**(*act*)

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

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

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

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

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

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

cogdl.utils.**args**

CHAPTER

SEVEN

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PYTHON MODULE INDEX

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