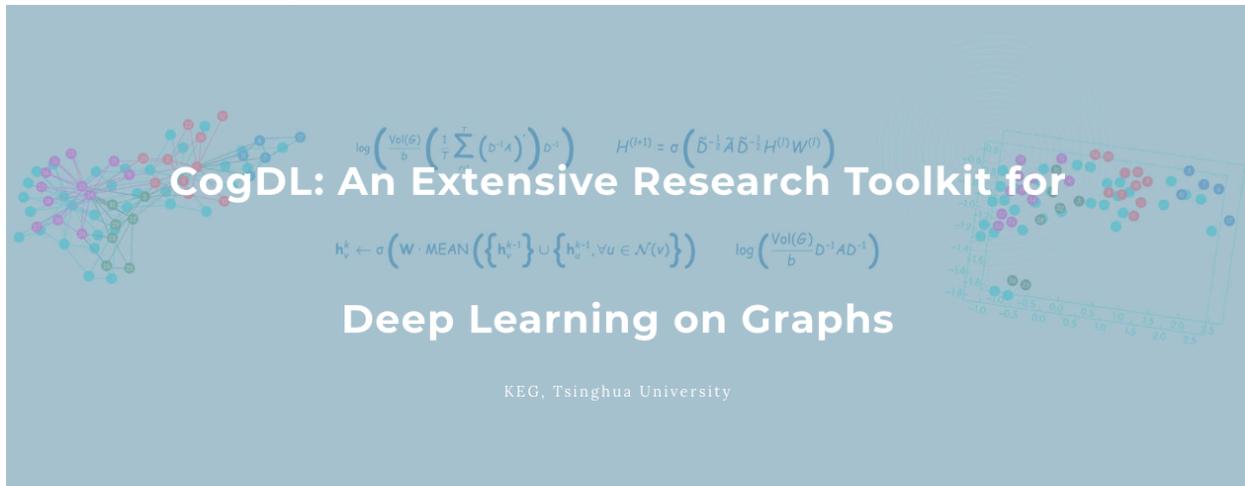

CogDL Documentation

KEG

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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)

INSTALL

- PyTorch version $\geq 1.0.0$
- 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 .
```


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 `cogdl/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 coresponding 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)
```

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 logistic 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 multilabel 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

- Set up “SupervisedGraphClassification” class, which has two specific parameters.
 - degree-feature*: Use one-hot node degree as node feature, for datasets such as Imdb-binary and Imdb-multi, which don't have node features.
 - gamma*: Multiplicative factor of learning rate decay.
 - lr*: Learning rate.
- 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
...
```

- 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 Imdb-binary and Imdb-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_percent:
        for shuf in shuffles:
            # ...
            clf = SVC()
            clf.fit(X_train, y_train)
            preds = clf.predict(X_test)

```

(continues on next page)

```
... # ...
```

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

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- [Zhang et al. (2019): ProNE: Fast and Scalable Network Representation Learning](<https://www.overleaf.com/read/dhgpkyfhdhj>)
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API REFERENCE

This page contains auto-generated API reference documentation¹.

6.1 cogdl

6.1.1 Subpackages

`cogdl.data`

Submodules

`cogdl.data.batch`

Module Contents

Classes

<i>Batch</i>	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

<i>Data</i>	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 extended 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.data_loader`

Module Contents

Classes

<code>DataLoader</code>	Data loader which merges data objects from a
<code>DataListLoader</code>	Data loader which merges data objects from a
<code>DenseDataLoader</code>	Data loader which merges data objects from a

class `cogdl.data.data_loader.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 many 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.data_loader.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 many 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.data_loader.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 many 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

<code>Dataset</code>	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

<code>download_url(url, folder, name=None, log=True)</code>	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

<code>maybe_log(path, log=True)</code>	
--	--

<code>extract_tar(path, folder, mode='r:gz', log=True)</code>	Extracts a tar archive to a specific folder.
---	--

<code>extract_zip(path, folder, log=True)</code>	Extracts a zip archive to a specific folder.
--	--

<code>extract_bz2(path, folder, log=True)</code>	
--	--

<code>extract_gz(path, folder, log=True)</code>	
---	--

`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

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

continues on next page

Table 10 – continued from previous page

<code>DataLoader</code>	Data loader which merges data objects from a
<code>DataListLoader</code>	Data loader which merges data objects from a
<code>DenseDataLoader</code>	Data loader which merges data objects from a

Functions

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

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 extended 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 many 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 many 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 many 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.ProteinsDataset`
Bases: `dgl.data.tu.TUDataset`

`cogdl.datasets.gatne`

Module Contents

Classes

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

Functions

<code>read_gatne_data(folder)</code>

`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

<code>Edgelist</code>	Dataset base class for creating graph datasets.
<code>USAAirportDataset</code>	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

<code>GTNDataset</code>	The network datasets “ACM”, “DBLP” and “IMDB” from the
<code>ACM_GTNDataset</code>	The network datasets “ACM”, “DBLP” and “IMDB” from the
<code>DBLP_GTNDataset</code>	The network datasets “ACM”, “DBLP” and “IMDB” from the
<code>IMDB_GTNDataset</code>	The network datasets “ACM”, “DBLP” and “IMDB” from the

Functions

<code>untar(path, fname, deleteTar=True)</code>	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

<i>HANDataset</i>	The network datasets “ACM”, “DBLP” and “IMDB” from the
<i>ACM_HANDataset</i>	The network datasets “ACM”, “DBLP” and “IMDB” from the
<i>DBLP_HANDataset</i>	The network datasets “ACM”, “DBLP” and “IMDB” from the
<i>IMDB_HANDataset</i>	The network datasets “ACM”, “DBLP” and “IMDB” from the

Functions

<i>untar</i> (path, fname, deleteTar=True)	Unpacks the given archive file to the same directory, then (by default)
<i>sample_mask</i> (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.

FB13Dataset

Dataset base class for creating graph datasets.

FB15kDataset

Dataset base class for creating graph datasets.

FB15k237Dataset

Dataset base class for creating graph datasets.

WN18Dataset

Dataset base class for creating graph datasets.

WN18RRDataset

Dataset base class for creating graph datasets.

FB13SDataset

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.FB13Dataset`

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.FB15kDataset`

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.FB15k237Dataset`

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.WN18Dataset`

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.FB13SDataset`

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

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

continues on next page

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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

continues on next page

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

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

Functions

<code>nx_to_graph_data_obj(g, center_id, allowable_features_downstream=None, allowable_features_pretrain=None, node_id_to_go_labels=None)</code>	
<code>graph_data_obj_to_nx(data)</code>	
<code>graph_data_obj_to_nx_simple(data)</code>	Converts graph Data object required by the pytorch geometric package to
<code>nx_to_graph_data_obj_simple(G)</code>	Converts nx graph to pytorch geometric Data object. Assume node indices
<code>reset_idxes(G)</code>	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 (ll, center=True)`

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

`__repr__ (self)`
Return repr(self).

class `cogdl.datasets.pyg_strategies_data.ChemExtractSubstructureContextPair (k, ll, 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,          trans-  
                                                    form=None,  
                                                    pre_transform=None,  
                                                    pre_filter=None)
```

Bases: torch_geometric.data.InMemoryDataset

```
class cogdl.datasets.pyg_strategies_data.TestChemDataset (data_type='unsupervised',  
                                                    root=None,          trans-  
                                                    form=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

<i>Dataset</i>	Dataset base class for creating graph datasets.
----------------	---

Functions

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

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

```
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

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

Functions

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

`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 adjacency 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 adjacency 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  $x = W[\text{node\_type}] * \text{gelu}(\text{Agg}(x)) + x$ 
    __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, source_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 sampled 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

<i>SELayer</i>	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', *in-*
put_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

<code>DeepGraphKernel</code>	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

<code>DistMult</code>	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)<<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

<code>GraRep</code>	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 transition 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

<code>Hin2vec_layer</code>	
<code>RWgraph</code>	
<code>Hin2vec</code>	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`

regular_tion (*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 negative 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

<i>Metapath2vec</i>	The Metapath2vec model from the "metapath2vec: Scalable Representation Learning for Heterogeneous Networks" paper
---------------------	---

```

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

<i>NetMF</i>	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

<i>NetSMF</i>	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

<i>ProNE</i>	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

<i>PTE</i>	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

<i>RotatE</i>	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

<i>SDNE_layer</i>	
-------------------	--

<i>SDNE</i>	The SDNE model from the “Structural Deep Network Embedding”
-------------	---

```
class cogdl.models.emb.sdne.SDNE_layer (num_node, hidden_size1, hidden_size2, dropout, 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, dropout, 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. `dropout` (float) : Dropout 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)” <<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

<code>GraphConvolution</code>	Simple GCN layer, similar to https://arxiv.org/abs/1609.02907
<code>ASGCN</code>	

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 sparsensor

_sample_one_layer (*self*, *x*, *adj*, *v*, *sample_size*)

sampling (*self*, *x*, *v*)

forward (*self*, *x*, *adj*)

`cogdl.models.nn.compvcn`

Module Contents

Classes

BasesRelEmbLayer

CompGCNLayer

CompGCN

LinkPredictCompGCN

Functions

<code>com_mult(a, b)</code>	Borrowed	from	https://github.com/malllabiisc/CompGCN
<code>conj(a)</code>	Borrowed	from	https://github.com/malllabiisc/CompGCN
<code>ccorr(a, b)</code>	Borrowed	from	https://github.com/malllabiisc/CompGCN

`cogdl.models.nn.compvcn.com_mult(a, b)`
 Borrowed from <https://github.com/malllabiisc/CompGCN>

`cogdl.models.nn.compvcn.conj(a)`
 Borrowed from <https://github.com/malllabiisc/CompGCN>

`cogdl.models.nn.compvcn.ccorr(a, b)`
 Borrowed from <https://github.com/malllabiisc/CompGCN>

class `cogdl.models.nn.compvcn.BasesRelEmbLayer` (*num_bases, num_rels, in_feats*)

Bases: `torch.nn.Module`

reset_parameters (*self*)

forward (*self*)

class `cogdl.models.nn.compvcn.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.compvcn.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

<code>preprocess_features(features)</code>	Row-normalize feature matrix and convert to tuple representation
<code>normalize_adj(adj)</code>	Symmetrically normalize adjacency matrix.
<code>sparse_mx_to_torch_sparse_tensor(sparse_mx)</code>	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_decomposition(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_decomposition(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, posi-
                                                    tional_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

<i>DisenGCNLayer</i>	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

<code>GraphConvolution</code>	Simple GCN layer, similar to https://arxiv.org/abs/1609.02907
<code>FastGCN</code>	

```
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

<i>SpecialSpmFunction</i>	Special function for only sparse region backpropataion layer.
<i>SpecialSpm</i>	
<i>SpGraphAttentionLayer</i>	Sparse version GAT layer, similar to https://arxiv.org/abs/1710.10903
<i>PetarVSpGAT</i>	The GAT model from the “Graph Attention Networks”

class `cogdl.models.nn.gat.SpecialSpmFunction`

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.SpecialSpm`

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

<code>GraphConvolution</code>	Simple GCN layer, similar to https://arxiv.org/abs/1609.02907
<code>TKipfGCN</code>	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

<code>GCNIILayer</code>
<code>GCNII</code>

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

<i>preprocess_features</i> (features)	Row-normalize feature matrix and convert to tuple representation
<i>normalize_adj</i> (adj)	Symmetrically normalize adjacency matrix.
<i>sparse_mx_to_torch_sparse_tensor</i> (sparse_mx)	Convert a scipy sparse matrix to a torch sparse tensor.
<i>compute_ppr</i> (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

<code>PatchySAN</code>	The Patchy-SAN model from the “Learning Convolutional Neural Networks for Graphs”
------------------------	---

Functions

<code>assemble_neighbor</code> (<i>G</i> , <i>node</i> , <i>num_neighbor</i> , <i>sorted_nodes</i>)	assemble neighbors for node with BFS strategy
<code>cmp</code> (<i>s1</i> , <i>s2</i>)	
<code>one_dim_wl</code> (<i>graph_list</i> , <i>init_labels</i> , <i>iteration=5</i>)	1-dimension WL method used for node normalization for all the subgraphs
<code>node_selection_with_1d_wl</code> (<i>G</i> , <i>features</i> , <i>num_channel</i> , <i>num_sample</i> , <i>num_neighbor</i> , <i>stride</i>)	construct features for cnn
<code>get_single_feature</code> (<i>data</i> , <i>num_features</i> , <i>num_classes</i> , <i>num_sample</i> , <i>num_neighbor</i> , <i>stride=1</i>)	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 nearest 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

<i>EntropyLoss</i>	
<i>LinkPredLoss</i>	
<i>GraphSAGE</i>	GraphSAGE from “Inductive Representation Learning on Large Graphs”.
<i>BatchedGraphSAGE</i>	GraphSAGE with mini-batch
<i>BatchedDiffPoolLayer</i>	DIFFPOOL from paper “Hierarchical Graph Representation Learning
<i>BatchedDiffPool</i>	DIFFPOOL layer with batch forward
<i>DiffPool</i>	DIFFPOOL from paper “Hierarchical Graph Representation Learning

Functions

<i>toBatchedGraph</i> (<i>batch_adj</i> , <i>batch_feat</i> , <i>node_per_pool_graph</i>)

```

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::  $h^{i+1}_{\mathcal{N}(v)} = \text{AGGREGATE}_{\{k\}}(h_{\mathcal{U}}^k) \oplus h^{k+1}_{\mathcal{V}}$ 
            $= \text{sigma}(\mathbf{W}^k \cdot \text{CONCAT}(h_{\mathcal{V}}^k, h_{\mathcal{N}(v)}))$ 

```

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) : Normalize 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, optional] 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 embedded 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 pooling 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

<code>GINLayer</code>	Graph Isomorphism Network layer from paper “How Powerful are Graph
<code>GINMLP</code>	Multilayer perception with batch normalization
<code>GIN</code>	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?”.

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

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

*MLP*Layer

Grand

class `cogdl.models.nn.pyg_grand.MLP`Layer(*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_dropout, hidden_dropout, use_bn, dropout_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

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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

<i>SUPEncoder</i>	Encoder used in supervised model with Set2set in paper “Order Matters: Sequence to sequence for sets”
<i>Encoder</i>	Encoder stacked with GIN layers
<i>FF</i>	Residual MLP layers.
<i>InfoGraph</i>	Implimentation of Infograph in paper “InfoGraph: Un-supervised 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:: $out = \text{mathbf{MLP}}(x) + \text{mathbf{Linear}}(x)$

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) <<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, atten-
                                         tion, 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

<i>SupervisedModel</i>	Helper class that provides a standard way to create an ABC using
<i>SupervisedHeterogeneousNodeClassification</i>	Helper class that provides a standard way to create an ABC using
<i>SupervisedHomogeneousNodeClassification</i>	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

<code>register_model(name)</code>	New model types can be added to cogdl with the <code>register_model()</code>
<code>alias_setup(probs)</code>	Compute utility lists for non-uniform sampling from discrete distributions.
<code>alias_draw(J, q)</code>	Draw sample from a non-uniform discrete distribution using alias sampling.
<code>build_model(args)</code>	

```
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

<code>GraphClassification</code>	Supervised graph classification task.
----------------------------------	---------------------------------------

Functions

<code>node_degree_as_feature(data)</code>	Set each node feature as one-hot encoding of degree
<code>uniform_node_feature(data)</code>	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`

Supervised 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

<code>HeterogeneousNodeClassification</code>	Heterogeneous Node classification task.
--	---

class `cogdl.tasks.heterogeneous_node_classification.HeterogeneousNodeClassification` (*args*,
dataset=None,
model=None)

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 *KnowledgeGraphEmbed-*
ding<<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/KnowledgeGraphEmbedding>>

```
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[SupervisedHomogeneousNodeClassification]
                                                    = 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

<i>NodeClassificationSampling</i>	Node classification task with sampling.
-----------------------------------	---

Functions

<i>get_batches</i> (train_nodes, batch_size=64, shuffle=True)	train_labels,
---	---------------

```
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=

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=None,
                                                                    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

<i>register_task</i> (name)	New task types can be added to cogdl with the <i>register_task()</i>
-----------------------------	--

<i>build_task</i> (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

<i>node_classification_sample</i> (<i>args, target_type, seed, nodes, time_range</i>)	tar-	sub-graph sampling and label preparation for node classification:
<i>prepare_data</i> (<i>args, graph, target_type, train_target_nodes, valid_target_nodes, pool</i>)		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)`

continues on next page

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<code>row_normalization(num_nodes, edge_index, edge_weight=None)</code>	
<code>symmetric_normalization(num_nodes, edge_index, edge_weight=None)</code>	
<code>sppmm(indices, values, b)</code>	Args:
<code>sppmm_adj(indices, values, shape, b)</code>	
<code>get_degrees(indices, num_nodes=None)</code>	
<code>edge_softmax(indices, values, shape)</code>	Args:
<code>mul_edge_softmax(indices, values, shape)</code>	Args:
<code>remove_self_loops(indices)</code>	
<code>get_activation(act)</code>	
<code>cycle_index(num, shift)</code>	
<code>batch_sum_pooling(x, batch)</code>	
<code>batch_mean_pooling(x, batch)</code>	
<code>tabulate_results(results_dict)</code>	
<code>print_result(results, datasets, model_name)</code>	
<code>set_random_seed(seed)</code>	

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.sppmm(indices, values, b)`

Args: indices : Tensor, shape=(2, E) values : Tensor, shape=(E,) shape : tuple(int, int) b : Tensor, shape=(N,)

`cogdl.utils.sppmm_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`

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