Big Graph Dataset Documentation

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Author Name

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Examples:

This is a collaboration project to build a large, multi-domain set of graph datasets. Each dataset comprises many small graphs.

The aim of this project is to provide a large set of graph datasets for use in machine learning research. Currently graph datasets are distributed in individual repositories, increasing workload as researchers have to search for relevant resources. Once these datasets are found, there is additional labour in formatting the data for use in deep learning.

We aim to provide datasets that are:

- Composed of many small graphs
- Diverse in domain
- Diverse in tasks
- Well-documented
- Formatted uniformly across datasets for Pytorch Geometric

1 Contributing

The GitHub repo can be found at *https://github.com/neutralpronoun/big-graph-dataset*.

The basics:

- Create your own git branch
- Copy the *datasets/example_dataset.py*
- Have a look through
- Re-tool it for your own dataset

I've provided code for sub-sampling graphs and producing statistics.

A few rules, demonstrated in *datasets/example_dataset.py*:

- The datasets need at least a train/val/test split
- Datasets should be many small (less than 400 node) graphs
- Ideally the number of graphs in each dataset should be controllable
- Data should be downloaded in-code to keep the repo small. If this isn't possible let me know.
- Please cite your sources for data in documentation - see the existing datasets for example documentation
- Where possible start from existing datasets that have been used in-literature, or if using generators, use generators that are well-understood (for example Erdos-Renyi graphs)

2 Getting Started

Check out the Reddit dataset example notebook for a quick start guide, then have a look at the source code for the datasets.

My environment is under *docs/requirements.txt*, use *pip install -r requirements. txt* within a virtual (Conda etc.) environment to get everything installed.

2.1 Reddit Example Dataset

A walkthrough of the dataset code for the Big Graph Dataset project

Alex Davies, University of Bristol, 2024

In this notebook we'll write code to:

- download a large Reddit graph from an online repository
- sample that graph to produce a dataset of smaller graphs
- process that dataset into a Pytorch Geometric InMemoryDataset

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Getting the graph

First we need to download the graph, here from the Stanford Network Analysis Project

We first find the links for the graph and node features (here node features are text embeddings):

[1]:
```
graph_url = "https://snap.stanford.edu/data/soc-redditHyperlinks-title.tsv"
embedding_url = "http://snap.stanford.edu/data/web-redditEmbeddings-subreddits.csv"
```

Then play with directories and download the data:

[2]:
```
import os
import pickle
import wget
import pandas as pd

# Swap into dataset directory
print(os.getcwd())
start_dir = os.getcwd()
os.chdir("original_datasets")

# We won't actually need this part in the final function!
if "reddit" not in os.listdir():
    os.mkdir("reddit")

os.chdir("reddit")

#  Download raw files if we don't already have them
if "soc-redditHyperlinks-title.tsv" not in os.listdir():
    graph_data = wget.download(graph_url) # Edgelist and edge features
if "web-redditEmbeddings-subreddits.csv" not in os.listdir():
    embedding_data = wget.download(embedding_url) # Node features

# We know that there are 300 components in the node feature vectors
embedding_column_names = ["COMPONENT", *[i for i in range(300)]]
embeddings = pd.read_csv("web-redditEmbeddings-subreddits.csv", names=embedding_
↪column_names).transpose()
graph_data = pd.read_csv("soc-redditHyperlinks-title.tsv", sep = "\t")


# Avoids weird directory problems
os.chdir(start_dir)
```

```
/home/alex/Projects/big-graph-dataset
```

Let's have a look at the node embeddings:

[3]:
```
embeddings.head()
```

[3]:
```
              0          1                    2          3         4      \
COMPONENT   spiders  askreddit  globaloffensivetrade  fireteams     funny
0          0.158972  -0.499114             -0.023145   2.492506  -0.81937
1          0.285813   0.323983             -1.199374  -2.529917 -0.865261
2          0.226329  -0.424809              1.661484  -0.448484  0.301753
3         -0.183338  -0.222705             -1.025296  -3.543441  0.018787

                5         6         7                8      \
```

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```
COMPONENT  the_donald    videos      news  leagueoflegends
0           -0.123265  0.131896  0.132825        -2.785298
1           -0.610208  0.866419  1.505527        -0.166391
2            0.361495  0.919025  0.730393         1.592624
3           -1.171773 -0.765584 -0.505759        -1.269829

                          9      …       51268              51269  \
COMPONENT  rocketleagueexchange  …  motleyfool  govtjobsrchinindia
0                     0.553341  …    0.004494            0.001908
1                    -3.283354  …    0.052268            0.042618
2                    -3.091485  …   -0.027792           -0.021329
3                     0.877085  …    0.013468               0.012

               51270     51271                51272     51273          51274  \
COMPONENT  snoopdogg   fortean  whatcanidoforbernie      33rd  bestofvic2015
0           -0.000534  0.000615             0.000906 -0.000076      -0.000203
1            0.023619  0.023847             0.017816 -0.001643       0.012698
2           -0.003317 -0.018297            -0.004231 -0.002896      -0.007575
3            0.005566 -0.004873            -0.010438  0.000581       0.006486

                51275           51276     51277
COMPONENT  aberystwyth  mail_forwarding     cover
0            -0.001563         0.009269   0.00457
1             0.004733         0.024779  0.012403
2            -0.000082        -0.017018 -0.000363
3            -0.000982        -0.007228 -0.002496

[5 rows x 51278 columns]
```

And now the edges:

[4]:
```
graph_data.head()
```

[4]:
```
    SOURCE_SUBREDDIT TARGET_SUBREDDIT  POST_ID            TIMESTAMP  \
0         rddtgaming         rddtrust  1u4pzzs  2013-12-31 16:39:18
1            xboxone    battlefield_4  1u4tmfs  2013-12-31 17:59:11
2                ps4    battlefield_4  1u4tmos  2013-12-31 17:59:40
3  fitnesscirclejerk        leangains  1u50xfs  2013-12-31 19:01:56
4  fitnesscirclejerk      lifeprotips  1u51nps  2013-12-31 21:02:28

   LINK_SENTIMENT                                          PROPERTIES
0               1  25.0,23.0,0.76,0.0,0.44,0.12,0.12,4.0,4.0,0.0,…
1               1  100.0,88.0,0.78,0.02,0.08,0.13,0.07,16.0,16.0,…
2               1  100.0,88.0,0.78,0.02,0.08,0.13,0.07,16.0,16.0,…
3               1  49.0,43.0,0.775510204082,0.0,0.265306122449,0…
4               1  14.0,14.0,0.785714285714,0.0,0.428571428571,0…
```

Turn the data into a graph

Now we need to turn the data into a graph. Our edges come from graph_data (SOURCE and TARGET), including categories for each edge (LINK_SENTIMENT), as well as edge features (PROPERTIES).

The first step is making a networkx.Graph object, which is a useful graph class, then we add the nodes one by one. We'll include the text embedding for the subreddit as a node attribute, taken from the embedding dataframe.

[5]:
```
# networkx is a Python library for graph structures
import networkx as nx
# tqdm for loading bars
from tqdm import tqdm
# cheeky function to visualise a networkx graph
from utils import vis_networkx

embeddings.columns = embeddings.iloc[0]
embeddings = embeddings.drop(["COMPONENT"], axis = 0)

graph = nx.Graph()

# Add a node for each id in the embedding data
for col in tqdm(embeddings.columns, desc = "Adding nodes"):
    # attrs here is taken from the embedding data, with the node id the column (col)
    graph.add_node(col, attrs=embeddings[col].to_numpy().astype(float))
```

```
Adding nodes: 100%|██████████| 51278/51278 [00:01<00:00, 32961.66it/s]
```

Now we add the edges (the actual graph stuff).

We need to include two properties:

- Type of edge, negative or positive interaction, -1 or 1. In dataframe as LINK_SENTIMENT
- Properties of the edge, text embedding of the reddit post content

[6]:
```
import numpy as np

def fix_property_string(input_string):
    input_string = input_string.split(',')
    input_string = [float(item) for item in input_string]

    return np.array(input_string)

sources = graph_data["SOURCE_SUBREDDIT"].to_numpy()
targets = graph_data["TARGET_SUBREDDIT"].to_numpy()

# This line can take a while!
attrs = [fix_property_string(properties) for properties in tqdm(graph_data["PROPERTIES
↪"].tolist(), desc = "Wrangling edge features")]
```

```
Wrangling edge features: 100%|██████████| 571927/571927 [00:05<00:00, 103705.47it/s]
```

Now iterate over the edges, only adding them if their nodes have data:

[7]:
```

labels = graph_data["LINK_SENTIMENT"].to_numpy()
all_nodes = list(graph.nodes())

for i in tqdm(range(sources.shape[0]), desc = "Adding edges"):
```

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```
    # Check that the edge has data
    if sources[i] in all_nodes and targets[i] in all_nodes:
        graph.add_edge(sources[i], targets[i],
                       labels = labels[i],
                       attr = attrs[i])
```

```
Adding edges: 100%|██████████| 571927/571927 [00:37<00:00, 15434.45it/s]
```

[8]:
```
print(graph)

# Last tidying bits
graph = nx.convert_node_labels_to_integers(graph)
CGs = [graph.subgraph(c) for c in nx.connected_components(graph)]
CGs = sorted(CGs, key=lambda x: x.number_of_nodes(), reverse=True)
graph = CGs[0]
graph = nx.convert_node_labels_to_integers(graph)

# Save the graph!
with open("original_datasets/reddit/reddit-graph.npz", "wb") as f:
    pickle.dump(graph, f)
```

```
Graph with 51278 nodes and 178143 edges
```

Nice! Graph achieved. Spot that in the last section we had to deal with some missing data - we're including edges ONLY if their nodes also have data.

Sample to make a dataset of smaller graphs

This is not too hard, I've written some code (Exploration Sampling With Replacement, ESWR) that does the sampling for you.

This will produce a big list of small networkx graphs sampled from that original graph.

[9]:
```
from utils import ESWR

# Sample 1000 graphs of max 96 nodes from the big reddit graph
nx_graph_list = ESWR(graph, 1000, 96)
```

```

Sampling 1000 in 5 chunks with size 200
```

```
Sampling from large graph: 100%|██████████| 6/6 [00:07<00:00,  1.31s/it]
```

```
Done sampling!


```

Next we need to convert it to a Pytorch Geometric format. This will be specific to your data - here we have node labels, edge labels, edge attributes.

[10]:
```
import torch
from torch_geometric.data import Data

def specific_from_networkx(graph):
    # Turns a graph into a pytorch geometric object
```

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```
    # Mostly by unpacking dictionaries on nodes and edges
    # Here node labels are the target
    # One of these functions for each dataset ideally - they are unlikely to transfer␣
↪across datasets
    node_attrs = []
    edge_indices = []
    edge_labels = []
    edge_attrs = []

    # Collect node labels and attributes
    for n in list(graph.nodes(data=True)):
        # list(graph.nodes(data=True)) returns [(node_id1, {attribute dictionary}),␣
↪(node_id2, ...), (node_id3, ...)]
        node_attrs.append(torch.Tensor(n[1]["attrs"]))

    # Collect edge indices and attributes
    for e in graph.edges(data=True):
        # graph.edges(data=True) is a generator producing (node_id1, node_id2,
↪{attribute dictionary})
        edge_indices.append((e[0], e[1]))

        edge_attrs.append(torch.Tensor(e[2]["attr"]))
        edge_labels.append(e[2]["labels"])


    # Specific to classification on edges! This is a binary edge classification (pos/
↪neg) task
    edge_labels = ((torch.Tensor(edge_labels) + 1)/2).reshape(-1,1)

    edge_attrs = torch.stack(edge_attrs)
    node_attrs = torch.stack(node_attrs)
    edge_indices = torch.tensor(edge_indices, dtype=torch.long).t().contiguous()

    # Create PyG Data object
    # Can pass:
    # x:            node features, shape (n nodes x n features)
    # edge_index:   the list of edges in the graph, shape (2, n_edges). Entries edge_
↪index[i, :] are [node_id1, node_id2].
    # edge_attr:    edge features, shape (n_edges, n_features), same order as edgelist
    # y:            targets. Graph regression shape (n_variables), graph␣
↪classification (n_classes), node classification (n_nodes, n_classes), edge␣
↪classification (n_edges, n_classes)
    data = Data(x=node_attrs, edge_index=edge_indices, edge_attr = edge_attrs, ␣
↪y=edge_labels)

    return data

print("Data in torch geometric format:")
specific_from_networkx(nx_graph_list[0])
```

```
Data in torch geometric format:
```

```
/home/alex/anaconda3/envs/adgcl/lib/python3.8/site-packages/tqdm/auto.py:21:␣
↪TqdmWarning: IProgress not found. Please update jupyter and ipywidgets. See https://
↪ipywidgets.readthedocs.io/en/stable/user_install.html
  from .autonotebook import tqdm as notebook_tqdm
```

[10]:
```
Data(x=[54, 300], edge_index=[2, 249], edge_attr=[249, 86], y=[249, 1])
```

The final dataset

Finally we place all that data into an InMemoryDataset!

Please note that in-code this whole notebook will be in functions - see `datasets/example_dataset.py`.

This means that the `datalist` argument wouldn't actually exist below - instead you'd call something like `get_reddit_dataset()` within your `.process` method.

[13]:
```
from torch_geometric.data import InMemoryDataset
from utils import vis_grid

class RedditDataset(InMemoryDataset):
    r"""
    Reddit hyperlink graphs - ie graphs of subreddits interacting with one another.
    The original graph is sourced from:

    `Kumar, Srijan, et al. "Community interaction and conflict on the web."
↪Proceedings of the 2018 world wide web conference. 2018.`

    The data has text embeddings as node features for each subreddit and text
↪features for the cross-post edges.

    The task is edge classification for the sentiment of the interaction between
↪subreddits.

    - Task: Edge classification
    - Num node features: 300
    - Num edge features: 86
    - Num target values: 1
    - Target shape: N Edges
    - Num graphs: Parameterised by `num`

    Args:
    root (str): Root directory where the dataset should be saved.
    datalist (list): A list of pytorch geometric data objects. Only obtained from an
↪argument here, not in actual code!
    stage (str): The stage of the dataset to load. One of "train", "val", "test".
↪(default: :obj:`"train"`)
    transform (callable, optional): A function/transform that takes in an :obj:`torch_
↪geometric.data.Data` object and returns a transformed version. The data object will
↪be transformed before every access. (default: :obj:`None`)
    pre_transform (callable, optional): A function/transform that takes in an :obj:
↪`torch_geometric.data.Data` object and returns a transformed version. The data
↪object will be transformed before being saved to disk. (default: :obj:`None`)
    pre_filter (callable, optional): A function that takes in an :obj:`torch_
↪geometric.data.Data` object and returns a boolean value, indicating whether the
↪data object should be included in the final dataset. (default: :obj:`None`)
    num (int): The number of samples to take from the original dataset. (default: :
↪obj:`2000`).
    """

    # datalist is only an argument for this notebook example - see existing datasets
↪under datasets/.. for how it actually works
    def __init__(self, root, datalist, stage = "train", transform=None, pre_
↪transform=None, pre_filter=None, num = 2000):
        self.num = num
        self.stage = stage
```

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```
        self.stage_to_index = {"train":0,
                               "val":1,
                               "test":2}
        self.datalist = datalist

        # Options are node-classification, node-regression, graph-classification,␣
↪graph-regression, edge-regression, edge-classification
        # Graph-level tasks are preferred! (graph-classification and graph-regression)
        # edge-prediction is another option if you can't think of a good task
        self.task = "node-classification"

        super().__init__(root, transform, pre_transform, pre_filter)
        self.data, self.slices = torch.load(self.processed_paths[self.stage_to_
↪index[self.stage]])


    @property
    def raw_file_names(self):
        # Replace with your saved raw file name
        return ['reddit-graph.npz']

    @property
    def processed_file_names(self):
        return ['train.pt',
                'val.pt',
                'test.pt']


    def process(self):
        # Read data into huge `Data` list.

        if os.path.isfile(self.processed_paths[self.stage_to_index[self.stage]]):
            print(f"Cora files exist")
            return

        # Get a list of num pytorch_geometric.data.Data objects
        data_list = self.datalist # get_example_dataset(num=self.num)

        # Torch geometric stuff
        if self.pre_filter is not None:
            data_list = [data for data in data_list if self.pre_filter(data)]

        if self.pre_transform is not None:
            data_list = [self.pre_transform(data) for data in data_list]

        # Save data
        data, slices = self.collate(data_list)
        torch.save((data, slices), self.processed_paths[self.stage_to_index[self.
↪stage]])

pyg_graphs = [specific_from_networkx(g) for g in tqdm(nx_graph_list, desc =
↪"Converting data to PyG data objects")]

# The visualisation doesn't work in documentation :( uncomment to see the graphs
vis_grid(pyg_graphs[:16], os.getcwd() + "/original_datasets/reddit/example.png", show_
↪plot = True)
```

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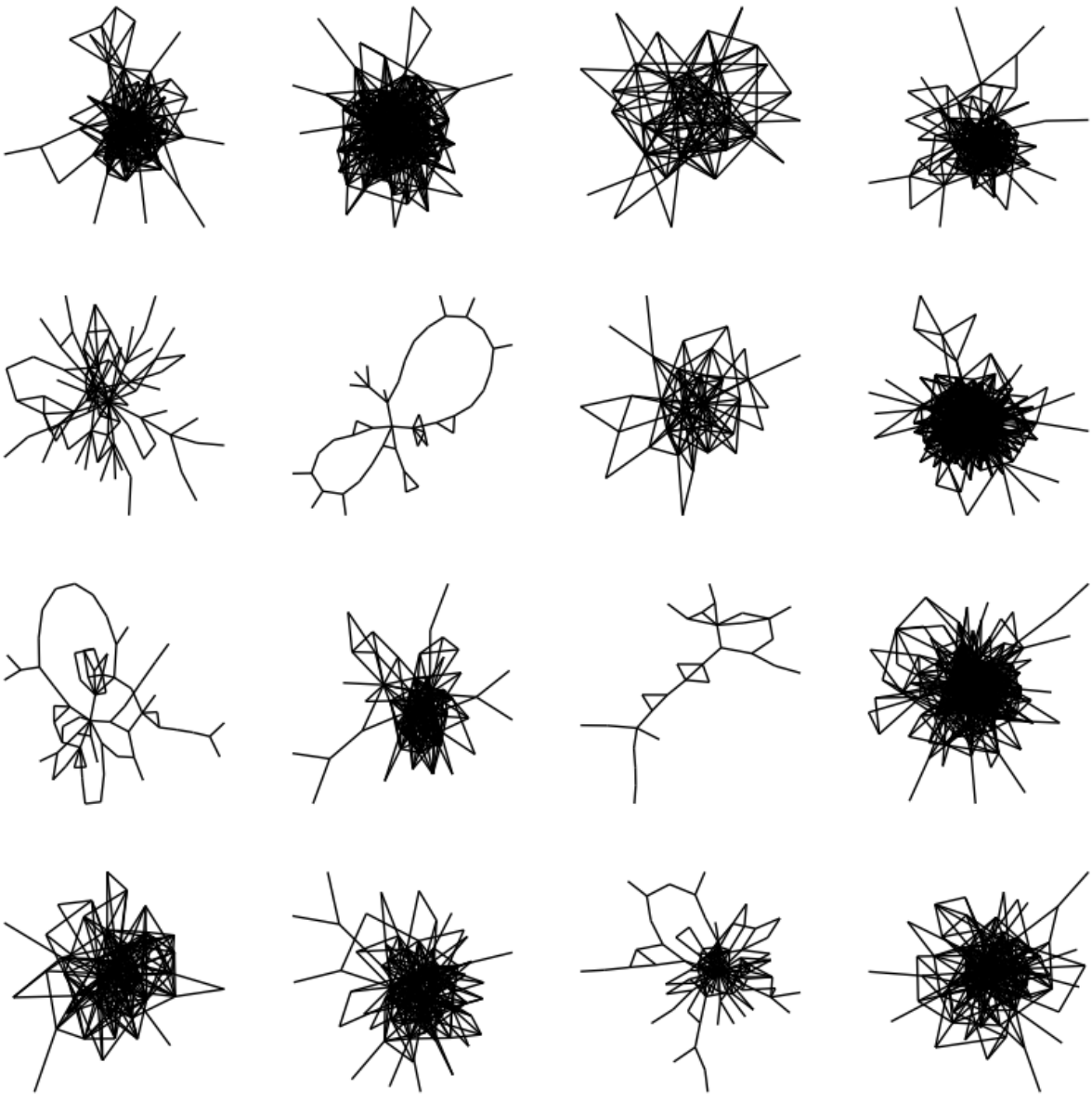
```
train_dataset = RedditDataset(os.getcwd() + "/original_datasets/reddit",
                              pyg_graphs)
```

```
Converting data to PyG data objects: 100%|██████████| 1000/1000 [00:01<00:00, 991.
↪15it/s]
/home/alex/Projects/big-graph-dataset/utils.py:398: UserWarning: The figure layout␣
↪has changed to tight
  plt.tight_layout()
```



```
Cora files exist
```

```
Processing...
Done!
```

Other datsets

There are already some datasets we can look at under datasets/DATASET.py.

3 Datasets

Documentation for the datsets currently in the Big Graph Dataset project.

3.1 Datasets

class datasets.**CoraDataset**(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

Bases: `InMemoryDataset`

Academic citation graphs from the ML community, sampled from a large original graph using ESWR. The original graph is sourced from:

> *Yang, Zhilin, William Cohen, and Ruslan Salakhudinov. "Revisiting semi-supervised learning with graph embeddings." International conference on machine learning. PMLR, 2016.*

The original data has one-hot bag-of-words over paper abstract as node features.

The task is node classification for the category of each paper, one-hot encoded for seven categories.

- Task: Node classification
- Num node features: 2879
- Num edge features: None
- Num target values: 7
- Target shape: N Nodes
- Num graphs: Parameterised by *num*

Parameters

- **root** (*str*) – Root directory where the dataset should be saved.
- **stage** (*str*) – The stage of the dataset to load. One of "train", "val", "test". (default: `"train"`)
- **transform** (*callable, optional*) – A function/transform that takes in an `torch_geometric.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 `torch_geometric.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 `torch_geometric.data.Data` object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: `None`)
- **num** (*int*) – The number of samples to take from the original dataset. (default: `2000`).

__init__(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

_abc_impl = <_abc._abc_data object>

_download()

_infer_num_classes(*y*)

Return type
int

_is_protocol = False

_process()

static collate(*data_list*)

Collates a Python list of `torch_geometric.data.Data` objects to the internal storage format of `InMemoryDataset`.

Return type
`Tuple[Data, Optional[Dict[str, Tensor]]]`

copy(*idx=None*)

Performs a deep-copy of the dataset. If `idx` is not given, will clone the full dataset. Otherwise, will only clone a subset of the dataset from indices `idx`. Indices can be slices, lists, tuples, and a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
InMemoryDataset

property data: Any

download()

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

get(*idx*)

Return type
Data

get_summary()

Collects summary statistics for the dataset.

property has_download: bool

Checks whether the dataset defines a *download()* method.

property has_process: bool

Checks whether the dataset defines a *process()* method.

index_select(*idx*)

Creates a subset of the dataset from specified indices `idx`. Indices `idx` can be a slicing object, *e.g.*, `[2:5]`, a list, a tuple, or a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
Dataset

indices()

Return type
Sequence

len()

Return type
int

property num_classes: int

property num_edge_features: int
Returns the number of features per edge in the dataset.

property num_features: int
Returns the number of features per node in the dataset. Alias for *num_node_features*.

property num_node_features: int
Returns the number of features per node in the dataset.

print_summary()
Prints summary statistics of the dataset to the console.

process()

property processed_dir: str

property processed_file_names

property processed_paths: List[str]
The absolute filepaths that must be present in order to skip processing.

property raw_dir: str

property raw_file_names

property raw_paths: List[str]
The absolute filepaths that must be present in order to skip downloading.

shuffle(*return_perm=False*)
Randomly shuffles the examples in the dataset.

Parameters
return_perm (*bool, optional*) – If set to `True`, will also return the random permutation used to shuffle the dataset. (default: `False`)

Return type
`Union`[`Dataset`, `Tuple`[`Dataset`, `Tensor`]]

to_datapipe()
Converts the dataset into a `torch.utils.data.DataPipe`.

The returned instance can then be used with **:pyg:`PyG's`** built-in `DataPipes` for baching graphs as follows:

```
from torch_geometric.datasets import QM9

dp = QM9(root='./data/QM9/').to_datapipe()
dp = dp.batch_graphs(batch_size=2, drop_last=True)

for batch in dp:
    pass
```

See the PyTorch tutorial for further background on DataPipes.

class datasets.**EgoDataset**(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=5000*)

Bases: InMemoryDataset

Ego networks from the streaming platform Twitch. The original graph is sourced from:

> *B. Rozemberczki, O. Kiss, R. Sarkar: An API Oriented Open-source Python Framework for Unsupervised Learning on Graphs 2019.*

The task is predicting whether a given streamer plays multiple different games.

- Task: Graph classification
- Num node features: None
- Num edge features: None
- Num target values: 1
- Target shape: 1
- Num graphs: 127094

Parameters

- **root** (*str*) – Root directory where the dataset should be saved.
- **stage** (*str*) – The stage of the dataset to load. One of "train", "val", "test". (default: "train")
- **transform** (*callable, optional*) – A function/transform that takes in an torch_geometric.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 torch_geometric.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 torch_geometric.data.Data object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: None)
- **num** (*int*) – The number of samples to take from the original dataset. (default: 2000).

__init__(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=5000*)

_abc_impl = <_abc._abc_data object>

_download()

_infer_num_classes(*y*)

Return type
int

_is_protocol = False

_process()

static collate(*data_list*)

Collates a Python list of torch_geometric.data.Data objects to the internal storage format of InMemoryDataset.

Return type
Tuple[Data, Optional[Dict[str, Tensor]]]

copy(*idx=None*)

Performs a deep-copy of the dataset. If `idx` is not given, will clone the full dataset. Otherwise, will only clone a subset of the dataset from indices `idx`. Indices can be slices, lists, tuples, and a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
InMemoryDataset

property data: Any

download()

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

get(*idx*)

Return type
Data

get_summary()

Collects summary statistics for the dataset.

property has_download: bool

Checks whether the dataset defines a *download()* method.

property has_process: bool

Checks whether the dataset defines a *process()* method.

index_select(*idx*)

Creates a subset of the dataset from specified indices `idx`. Indices `idx` can be a slicing object, *e.g.*, `[2:5]`, a list, a tuple, or a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
Dataset

indices()

Return type
Sequence

len()

Return type
int

property num_classes: int

property num_edge_features: int

Returns the number of features per edge in the dataset.

property num_features: int

Returns the number of features per node in the dataset. Alias for *num_node_features*.

property num_node_features: int

Returns the number of features per node in the dataset.

print_summary()

Prints summary statistics of the dataset to the console.

process()

property processed_dir: str

property processed_file_names

property processed_paths: List[str]

The absolute filepaths that must be present in order to skip processing.

property raw_dir: str

property raw_file_names

property raw_paths: List[str]

The absolute filepaths that must be present in order to skip downloading.

shuffle(*return_perm=False*)

Randomly shuffles the examples in the dataset.

Parameters

return_perm (*bool, optional*) – If set to `True`, will also return the random permutation used to shuffle the dataset. (default: `False`)

Return type

`Union`[`Dataset`, `Tuple`[`Dataset`, `Tensor`]]

to_datapipe()

Converts the dataset into a `torch.utils.data.DataPipe`.

The returned instance can then be used with **:pyg:`PyG's`** built-in `DataPipes` for baching graphs as follows:

```
from torch_geometric.datasets import QM9

dp = QM9(root='./data/QM9/').to_datapipe()
dp = dp.batch_graphs(batch_size=2, drop_last=True)

for batch in dp:
    pass
```

See the PyTorch tutorial for further background on DataPipes.

class datasets.**FacebookDataset**(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

Bases: `InMemoryDataset`

Facebook page-to-page interaction graphs, sampled from a large original graph using ESWR. The original graph is sourced from:

> *Benedek Rozemberczki, Carl Allen, and Rik Sarkar. Multi-Scale Attributed Node Embedding. Journal of Complex Networks 2021*

The original data has node features, but as they are of varying length, we don't include them here.

The task is node classification for the category of each Facebook page in a given graph, one-hot encoded for four categories.

- Task: Node classification
- Num node features: None
- Num edge features: None

- Num target values: 4
- Target shape: N Nodes
- Num graphs: Parameterised by *num*

Parameters

- **root** (*str*) – Root directory where the dataset should be saved.
- **stage** (*str*) – The stage of the dataset to load. One of "train", "val", "test". (default: `"train"`)
- **transform** (*callable, optional*) – A function/transform that takes in an `torch_geometric.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 `torch_geometric.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 `torch_geometric.data.Data` object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: `None`)
- **num** (*int*) – The number of samples to take from the original dataset. (default: `2000`).

__init__(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

_abc_impl = <_abc._abc_data object>

_download()

_infer_num_classes(*y*)

Return type
`int`

_is_protocol = False

_process()

static collate(*data_list*)

Collates a Python list of `torch_geometric.data.Data` objects to the internal storage format of `InMemoryDataset`.

Return type
`Tuple[Data, Optional[Dict[str, Tensor]]]`

copy(*idx=None*)

Performs a deep-copy of the dataset. If `idx` is not given, will clone the full dataset. Otherwise, will only clone a subset of the dataset from indices `idx`. Indices can be slices, lists, tuples, and a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
`InMemoryDataset`

property data: Any

download()

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

get(*idx*)

Return type
Data

get_summary()
Collects summary statistics for the dataset.

property has_download: bool
Checks whether the dataset defines a *download()* method.

property has_process: bool
Checks whether the dataset defines a *process()* method.

index_select(*idx*)
Creates a subset of the dataset from specified indices `idx`. Indices `idx` can be a slicing object, *e.g.*, `[2:5]`, a list, a tuple, or a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
Dataset

indices()

Return type
Sequence

len()

Return type
int

property num_classes: int

property num_edge_features: int
Returns the number of features per edge in the dataset.

property num_features: int
Returns the number of features per node in the dataset. Alias for *num_node_features*.

property num_node_features: int
Returns the number of features per node in the dataset.

print_summary()
Prints summary statistics of the dataset to the console.

process()

property processed_dir: str

property processed_file_names

property processed_paths: List[str]
The absolute filepaths that must be present in order to skip processing.

property raw_dir: str

property raw_file_names

property raw_paths: List[str]
The absolute filepaths that must be present in order to skip downloading.

shuffle(*return_perm=False*)

Randomly shuffles the examples in the dataset.

Parameters

return_perm (*bool, optional*) – If set to `True`, will also return the random permutation used to shuffle the dataset. (default: `False`)

Return type

`Union[Dataset, Tuple[Dataset, Tensor]]`

to_datapipe()

Converts the dataset into a `torch.utils.data.DataPipe`.

The returned instance can then be used with **:pyg:`PyG's`** built-in `DataPipes` for baching graphs as follows:

```
from torch_geometric.datasets import QM9

dp = QM9(root='./data/QM9/').to_datapipe()
dp = dp.batch_graphs(batch_size=2, drop_last=True)

for batch in dp:
    pass
```

See the PyTorch tutorial for further background on DataPipes.

class datasets.**NeuralDataset**(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

Bases: `InMemoryDataset`

A dataset of the connectome of a fruit fly larvae. The original graph is sourced from:

Michael Winding et al. , The connectome of an insect brain.Science379,eadd9330(2023).DOI:10.1126/science.add9330

We process the original multigraph into ESWR samples of this neural network, with predicting the strength of the connection (number of synapses) between two neurons as the target.

- Task: Edge regression
- Num node features: 0
- Num edge features: 0
- Num target values: 1
- Target shape: N Edges
- Num graphs: Parameterised by *num*

Parameters

- **root** (*str*) – Root directory where the dataset should be saved.
- **stage** (*str*) – The stage of the dataset to load. One of "train", "val", "test". (default: `"train"`)
- **transform** (*callable, optional*) – A function/transform that takes in an `torch_geometric.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 `torch_geometric.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 `torch_geometric.data.Data` object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: `None`)
- **num** (*int*) – The number of samples to take from the original dataset. (default: `2000`).

__init__(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

_abc_impl = <_abc._abc_data object>

_download()

_infer_num_classes(*y*)

Return type
`int`

_is_protocol = False

_process()

static collate(*data_list*)

Collates a Python list of `torch_geometric.data.Data` objects to the internal storage format of `InMemoryDataset`.

Return type
`Tuple[Data, Optional[Dict[str, Tensor]]]`

copy(*idx=None*)

Performs a deep-copy of the dataset. If `idx` is not given, will clone the full dataset. Otherwise, will only clone a subset of the dataset from indices `idx`. Indices can be slices, lists, tuples, and a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
`InMemoryDataset`

property data: Any

download()

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

get(*idx*)

Return type
`Data`

get_summary()

Collects summary statistics for the dataset.

property has_download: bool

Checks whether the dataset defines a *download()* method.

property has_process: bool

Checks whether the dataset defines a *process()* method.

index_select(*idx*)

Creates a subset of the dataset from specified indices `idx`. Indices `idx` can be a slicing object, *e.g.*, `[2:5]`, a list, a tuple, or a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
`Dataset`

indices()

Return type
Sequence

len()

Return type
int

property num_classes: int

property num_edge_features: int
Returns the number of features per edge in the dataset.

property num_features: int
Returns the number of features per node in the dataset. Alias for *num_node_features*.

property num_node_features: int
Returns the number of features per node in the dataset.

print_summary()
Prints summary statistics of the dataset to the console.

process()

property processed_dir: str

property processed_file_names

property processed_paths: List[str]
The absolute filepaths that must be present in order to skip processing.

property raw_dir: str

property raw_file_names

property raw_paths: List[str]
The absolute filepaths that must be present in order to skip downloading.

shuffle(*return_perm=False*)
Randomly shuffles the examples in the dataset.

Parameters
return_perm (*bool, optional*) – If set to True, will also return the random permutation used to shuffle the dataset. (default: False)

Return type
Union[Dataset, Tuple[Dataset, Tensor]]

to_datapipe()
Converts the dataset into a torch.utils.data.DataPipe.

The returned instance can then be used with **:pyg:`PyG's`** built-in DataPipes for baching graphs as follows:

```
from torch_geometric.datasets import QM9

dp = QM9(root='./data/QM9/').to_datapipe()
dp = dp.batch_graphs(batch_size=2, drop_last=True)
```

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```
for batch in dp:
    pass
```

See the PyTorch tutorial for further background on DataPipes.

class datasets.**RedditDataset**(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

Bases: InMemoryDataset

Reddit hyperlink graphs - ie graphs of subreddits interacting with one another. The original graph is sourced from:

> *Kumar, Srijan, et al. "Community interaction and conflict on the web." Proceedings of the 2018 world wide web conference. 2018.*

The data has text embeddings as node features for each subreddit and text features for the cross-post edges.

The task is edge classification for the sentiment of the interaction between subreddits.

- Task: Edge classification
- Num node features: 300
- Num edge features: 86
- Num target values: 1
- Target shape: N Edges
- Num graphs: Parameterised by *num*

Parameters

- **root** (*str*) – Root directory where the dataset should be saved.
- **stage** (*str*) – The stage of the dataset to load. One of "train", "val", "test". (default: "train")
- **transform** (*callable, optional*) – A function/transform that takes in an torch_geometric.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 torch_geometric.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 torch_geometric.data.Data object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: None)
- **num** (*int*) – The number of samples to take from the original dataset. (default: 2000).

__init__(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

_abc_impl = <_abc._abc_data object>

_download()

_infer_num_classes(*y*)

Return type
int

_is_protocol = False

_process()

static collate(*data_list*)

Collates a Python list of `torch_geometric.data.Data` objects to the internal storage format of `InMemoryDataset`.

Return type
`Tuple[Data, Optional[Dict[str, Tensor]]]`

copy(*idx=None*)

Performs a deep-copy of the dataset. If `idx` is not given, will clone the full dataset. Otherwise, will only clone a subset of the dataset from indices `idx`. Indices can be slices, lists, tuples, and a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
`InMemoryDataset`

property data: Any

download()

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

get(*idx*)

Return type
`Data`

get_summary()

Collects summary statistics for the dataset.

property has_download: bool

Checks whether the dataset defines a *download()* method.

property has_process: bool

Checks whether the dataset defines a *process()* method.

index_select(*idx*)

Creates a subset of the dataset from specified indices `idx`. Indices `idx` can be a slicing object, *e.g.*, `[2:5]`, a list, a tuple, or a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
`Dataset`

indices()

Return type
`Sequence`

len()

Return type
`int`

property num_classes: int

property num_edge_features: int

Returns the number of features per edge in the dataset.

property num_features: int

Returns the number of features per node in the dataset. Alias for *num_node_features*.

property num_node_features: int

Returns the number of features per node in the dataset.

print_summary()

Prints summary statistics of the dataset to the console.

process()

property processed_dir: str

property processed_file_names

property processed_paths: List[str]

The absolute filepaths that must be present in order to skip processing.

property raw_dir: str

property raw_file_names

property raw_paths: List[str]

The absolute filepaths that must be present in order to skip downloading.

shuffle(*return_perm=False*)

Randomly shuffles the examples in the dataset.

Parameters

return_perm (*bool, optional*) – If set to `True`, will also return the random permutation used to shuffle the dataset. (default: `False`)

Return type

`Union`[`Dataset`, `Tuple`[`Dataset`, `Tensor`]]

to_datapipe()

Converts the dataset into a `torch.utils.data.DataPipe`.

The returned instance can then be used with **:pyg:`PyG's`** built-in `DataPipes` for baching graphs as follows:

```
from torch_geometric.datasets import QM9

dp = QM9(root='./data/QM9/').to_datapipe()
dp = dp.batch_graphs(batch_size=2, drop_last=True)

for batch in dp:
    pass
```

See the PyTorch tutorial for further background on DataPipes.

class datasets.**RoadDataset**(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

Bases: `InMemoryDataset`

Road graphs from Pennsylvania, sampled from a large original graph using ESWR. The original graph is sourced from:

J. Leskovec, K. Lang, A. Dasgupta, M. Mahoney. Community Structure in Large Networks: Natural Cluster Sizes and the Absence of Large Well-Defined Clusters. Internet Mathematics 6(1) 29–123, 2009.

The task is predicting whether a given graph is planar (can be laid out with no crossing edges).

- Task: Graph classification
- Num node features: None
- Num edge features: None
- Num target values: 1
- Target shape: 1
- Num graphs: Parameterised by *num*

Parameters

- **root** (*str*) – Root directory where the dataset should be saved.
- **stage** (*str*) – The stage of the dataset to load. One of "train", "val", "test". (default: `"train"`)
- **transform** (*callable, optional*) – A function/transform that takes in an `torch_geometric.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 `torch_geometric.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 `torch_geometric.data.Data` object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: `None`)
- **num** (*int*) – The number of samples to take from the original dataset. (default: `2000`).

__init__(*root*, *stage='train'*, *transform=None*, *pre_transform=None*, *pre_filter=None*, *num=2000*)

_abc_impl = <_abc._abc_data object>

_download()

_infer_num_classes(*y*)

Return type
`int`

_is_protocol = False

_process()

static collate(*data_list*)

Collates a Python list of `torch_geometric.data.Data` objects to the internal storage format of `InMemoryDataset`.

Return type
`Tuple[Data, Optional[Dict[str, Tensor]]]`

copy(*idx=None*)

Performs a deep-copy of the dataset. If `idx` is not given, will clone the full dataset. Otherwise, will only clone a subset of the dataset from indices `idx`. Indices can be slices, lists, tuples, and a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
InMemoryDataset

property data: Any

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

get(*idx*)

Return type
Data

get_summary()
Collects summary statistics for the dataset.

property has_download: bool
Checks whether the dataset defines a *download()* method.

property has_process: bool
Checks whether the dataset defines a *process()* method.

index_select(*idx*)
Creates a subset of the dataset from specified indices `idx`. Indices `idx` can be a slicing object, *e.g.*, `[2:5]`, a list, a tuple, or a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
Dataset

indices()

Return type
Sequence

len()

Return type
int

property num_classes: int

property num_edge_features: int
Returns the number of features per edge in the dataset.

property num_features: int
Returns the number of features per node in the dataset. Alias for *num_node_features*.

property num_node_features: int
Returns the number of features per node in the dataset.

print_summary()
Prints summary statistics of the dataset to the console.

process()

property processed_dir: str

property processed_file_names

property processed_paths: List[str]

The absolute filepaths that must be present in order to skip processing.

property raw_dir: str

property raw_file_names

property raw_paths: List[str]

The absolute filepaths that must be present in order to skip downloading.

shuffle(*return_perm=False*)

Randomly shuffles the examples in the dataset.

Parameters

return_perm (*bool, optional*) – If set to `True`, will also return the random permutation used to shuffle the dataset. (default: `False`)

Return type

`Union`[`Dataset`, `Tuple`[`Dataset`, `Tensor`]]

to_datapipe()

Converts the dataset into a `torch.utils.data.DataPipe`.

The returned instance can then be used with **:pyg:`PyG's`** built-in `DataPipes` for baching graphs as follows:

```
from torch_geometric.datasets import QM9

dp = QM9(root='./data/QM9/').to_datapipe()
dp = dp.batch_graphs(batch_size=2, drop_last=True)

for batch in dp:
    pass
```

See the PyTorch tutorial for further background on DataPipes.

datasets.**get_all_datasets**(*transforms*, *num=5000*, *mol_only=False*)

datasets.**get_test_datasets**(*transforms*, *num=2000*, *mol_only=False*)

datasets.**get_train_datasets**(*transforms*, *num=2000*, *mol_only=False*)

datasets.**get_val_datasets**(*transforms*, *num=2000*, *mol_only=False*)

4 ToP (Topology Only Pre-Training)

Documentation for the Topology Only Pre-Training component of the project. We are using a pre-trained model to generate embeddings of the graphs in the datasets, hopefully to get some measure of how diverse the datasets are. Very much a work-in-progress!

4.1 ToP (Topology only Pre-training)

class top.**GeneralEmbeddingEvaluation**

Bases: object

Class for evaluating embeddings and visualizing the results.

__init__()

Initializes the GeneralEmbeddingEvaluation object.

embedding_evaluation(*encoder*, *train_loaders*, *names*)

Performs embedding evaluation using the given encoder, train loaders, and names.

get_embeddings(*encoder*, *loaders*, *names*)

Retrieves the embeddings from the encoder and loaders.

vis(*all_embeddings*, *separate_embeddings*, *names*)

Visualizes the embeddings using UMAP and PCA projections.

centroid_similarities(*embeddings*, *names*)

Calculates the pairwise similarities between the centroids of the embeddings.

__init__()

centroid_similarities(*embeddings*, *names*)

Calculate centroid similarities for a given set of embeddings and names.

Parameters: embeddings (list of numpy arrays): List of embeddings, where each embedding is a numpy array. names (list of str): List of names corresponding to the embeddings.

Returns: None

This method calculates the centroid similarities for a given set of embeddings. It first calculates the centroid for each embedding by taking the mean along the axis 0. Then, it calculates the pairwise similarities between the centroids using cosine similarity. Finally, it visualizes the pairwise similarities as a heatmap and saves the plot as "outputs/pairwise-similarity.png".

embedding_evaluation(*encoder*, *train_loaders*, *names*)

Evaluate the embeddings generated by the encoder.

Parameters

- **encoder** – The encoder model used to generate the embeddings.
- **train_loaders** – A list of data loaders for the data.
- **names** – A list of names corresponding to the data loaders.

Returns

None

get_embeddings(*encoder*, *loaders*, *names*)

Get embeddings for the given encoder and loaders.

Parameters

- **encoder** – The encoder model.
- **loaders** – A list of data loaders.
- **names** – A list of names corresponding to the loaders.

Returns
A tuple containing the concatenated embeddings of all loaders and a list of separate embeddings for each loader.

vis (*all_embeddings*, *separate_embeddings*, *names*)

Visualizes the embeddings using UMAP and PCA projections.

Parameters

- **all_embeddings** (*numpy.ndarray*) – The combined embeddings of all graphs.
- **separate_embeddings** (*list*) – A list of separate embeddings for each graph.
- **names** (*list*) – A list of names corresponding to each graph.

Returns
None

class top.**ToPDataset** (*root*, *original_dataset*, *num=-1*, *transform=None*, *pre_transform=None*, *pre_filter=None*)

Bases: InMemoryDataset

Processes an InMemoryDataset into a ToP dataset by removing node and edge features.

Based on the paper:

Towards Generalised Pre-Training of Graph Models, Davies, A. O., Green, R. W., Ajmeri, N. S., and Silva Filho, T. M., arXiv e-prints, 2024. doi:10.48550/arXiv.2311.03976.

The resulting dataset is topology-only, intended for pre-training with ToP, and as such this module does not produce validation/test splits.

Parameters

- **root** (*str*) – Root directory where the dataset should be saved. The dataset will be saved in *root*/train-top.pt
- **original_dataset** (*InMemoryDataset*) – The original dataset to convert to ToP format.
- **num** (*int*) – The number of samples to take from the original dataset. *num=-1* will convert all available samples from the original. (default: `-1`).
- **transform** (*callable, optional*) – A function/transform that takes in an `torch_geometric.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 `torch_geometric.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 `torch_geometric.data.Data` object and returns a boolean value, indicating whether the data object should be included in the final dataset. (default: `None`)

__init__ (*root*, *original_dataset*, *num=-1*, *transform=None*, *pre_transform=None*, *pre_filter=None*)

_abc_impl = <_abc._abc_data object>

_download()

_infer_num_classes(*y*)

Return type
int

_is_protocol = False

_process()

static collate(*data_list*)

Collates a Python list of `torch_geometric.data.Data` objects to the internal storage format of `InMemoryDataset`.

Return type
Tuple[Data, Optional[Dict[str, Tensor]]]

copy(*idx=None*)

Performs a deep-copy of the dataset. If `idx` is not given, will clone the full dataset. Otherwise, will only clone a subset of the dataset from indices `idx`. Indices can be slices, lists, tuples, and a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
InMemoryDataset

property data: Any

download()

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

get(*idx*)

Return type
Data

get_summary()

Collects summary statistics for the dataset.

property has_download: bool

Checks whether the dataset defines a *download()* method.

property has_process: bool

Checks whether the dataset defines a *process()* method.

index_select(*idx*)

Creates a subset of the dataset from specified indices `idx`. Indices `idx` can be a slicing object, *e.g.*, `[2:5]`, a list, a tuple, or a `torch.Tensor` or `np.ndarray` of type long or bool.

Return type
Dataset

indices()

Return type
Sequence

len()

Return type
int

property num_classes: int

property num_edge_features: int

Returns the number of features per edge in the dataset.

property num_features: int

Returns the number of features per node in the dataset. Alias for *num_node_features*.

property num_node_features: int

Returns the number of features per node in the dataset.

print_summary()

Prints summary statistics of the dataset to the console.

process()

property processed_dir: str

property processed_file_names

property processed_paths: List[str]

The absolute filepaths that must be present in order to skip processing.

property raw_dir: str

property raw_file_names

property raw_paths: List[str]

The absolute filepaths that must be present in order to skip downloading.

shuffle(*return_perm=False*)

Randomly shuffles the examples in the dataset.

Parameters

return_perm (*bool, optional*) – If set to `True`, will also return the random permutation used to shuffle the dataset. (default: `False`)

Return type

`Union`[`Dataset`, `Tuple`[`Dataset`, `Tensor`]]

to_datapipe()

Converts the dataset into a `torch.utils.data.DataPipe`.

The returned instance can then be used with **:pyg:`PyG's`** built-in `DataPipes` for baching graphs as follows:

```
from torch_geometric.datasets import QM9

dp = QM9(root='./data/QM9/').to_datapipe()
dp = dp.batch_graphs(batch_size=2, drop_last=True)

for batch in dp:
    pass
```

See the PyTorch tutorial for further background on DataPipes.

top.**compute_top_scores**(*datasets*, *names*)

Computes the top scores for graph structures using the ToP encoder.

ToP scores use a pre-trained ToP model to compute the similarity between graphs across datasets.

This function will also produce embedding visualisations using GeneralEmbeddingEvaluation.

Parameters

- **datasets** (*list*) – A list of datasets containing graph structures.
- **names** (*list*) – A list of names corresponding to each dataset.

Returns

None

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