7.1 Data Preprocessing

Before launching training jobs, DGL requires the input data to be partitioned and distributed to the target machines. In order to handle different scales of graphs, DGL provides 2 partitioning approaches:

- A partitioning API for graphs that can fit in a single machine memory.
- A distributed partition pipeline for graphs beyond a single machine capacity.

7.1.1 Partitioning API

For relatively small graphs, DGL provides a partitioning API `partition_graph()` that partitions an in-memory `DGLGraph` object. It supports multiple partitioning algorithms such as random partitioning and Metis. The benefit of Metis partitioning is that it can generate partitions with minimal edge cuts to reduce network communication for distributed training and inference. DGL uses the latest version of Metis with the options optimized for the real-world graphs with power-law distribution. After partitioning, the API constructs the partitioned results in a format that is easy to load during the training. For example,

```
import dgl

g = ...  # create or load a DGLGraph object
dgl.distributed.partition_graph(g, 'mygraph', 2, 'data_root_dir')
```

will outputs the following data file.

```
data_root_dir/
  |-- mygraph.json          # metadata JSON. File name is the given graph name.
  |-- part0/                # data for partition 0
  |   |-- node_feats.dgl    # node features stored in binary format
  |   |-- edge_feats.dgl    # edge features stored in binary format
  |   |-- graph.dgl         # graph structure of this partition stored in binary format
  |
  |-- part1/                # data for partition 1
      |-- node_feats.dgl
      |-- edge_feats.dgl
      |-- graph.dgl
```

Chapter 7.4 Advanced Graph Partitioning covers more details about the partition format. To distribute the partitions to a cluster, users can either save the data in some shared folder accessible by all machines, or copy the metadata JSON as well as the corresponding partition folder `partX` to the X^th machine.

Using `partition_graph()` requires an instance with large enough CPU RAM to hold the entire graph structure and features, which may not be viable for graphs with hundreds of billions of edges or large features. We describe how to use the *parallel data preparation pipeline* for such cases next.

Load balancing

When partitioning a graph, by default, METIS only balances the number of nodes in each partition. This can result in suboptimal configuration, depending on the task at hand. For example, in the case of semi-supervised node classification, a trainer performs computation on a subset of labeled nodes in a local partition. A partitioning that only balances nodes in a graph (both labeled and unlabeled), may end up with computational load imbalance. To get a balanced workload in each partition, the partition API allows balancing between partitions with respect to the number of nodes in each node type, by specifying `balance_ntypes` in `partition_graph()`. Users can take advantage of this and consider nodes in the training set, validation set and test set are of different node types.

The following example considers nodes inside the training set and outside the training set are two types of nodes:

```
dgl.distributed.partition_graph(g, 'graph_name', 4, '/tmp/test',
balance_ntypes=g.ndata['train_mask'])
```

In addition to balancing the node types, `dgl.distributed.partition_graph()` also allows balancing between in-degrees of nodes of different node types by specifying `balance_edges`. This balances the number of edges incident to the nodes of different types.

ID mapping

After partitioning, `partition_graph()` remap node and edge IDs so that nodes of the same partition are aranged together (in a consecutive ID range), making it easier to store partitioned node/edge features. The API also automatically shuffles the node/edge features according to the new IDs. However, some downstream tasks may want to recover the original node/edge IDs (such as extracting the computed node embeddings for later use). For such cases, pass `return_mapping=True` to `partition_graph()`, which makes the API returns the ID mappings between the remapped node/edge IDs and their origianl ones. For a homogeneous graph, it returns two vectors. The first vector maps every new node ID to its original ID; the

second vector maps every new edge ID to its original ID. For a heterogeneous graph, it returns two dictionaries of vectors. The first dictionary contains the mapping for each node type; the second dictionary contains the mapping for each edge type.

```
node_map, edge_map = dgl.distributed.partition_graph(g, 'graph_name', 4, '/tmp/test',
                                                     balance_ntypes=g.ndata['train_mask'],
                                                     return_mapping=True)
# Let's assume that node_emb is saved from the distributed training.
orig_node_emb = th.zeros(node_emb.shape, dtype=node_emb.dtype)
orig_node_emb[node_map] = node_emb
```

Load partitioned graphs

DGL provides a `dgl.distributed.load_partition()` function to load one partition for inspection.

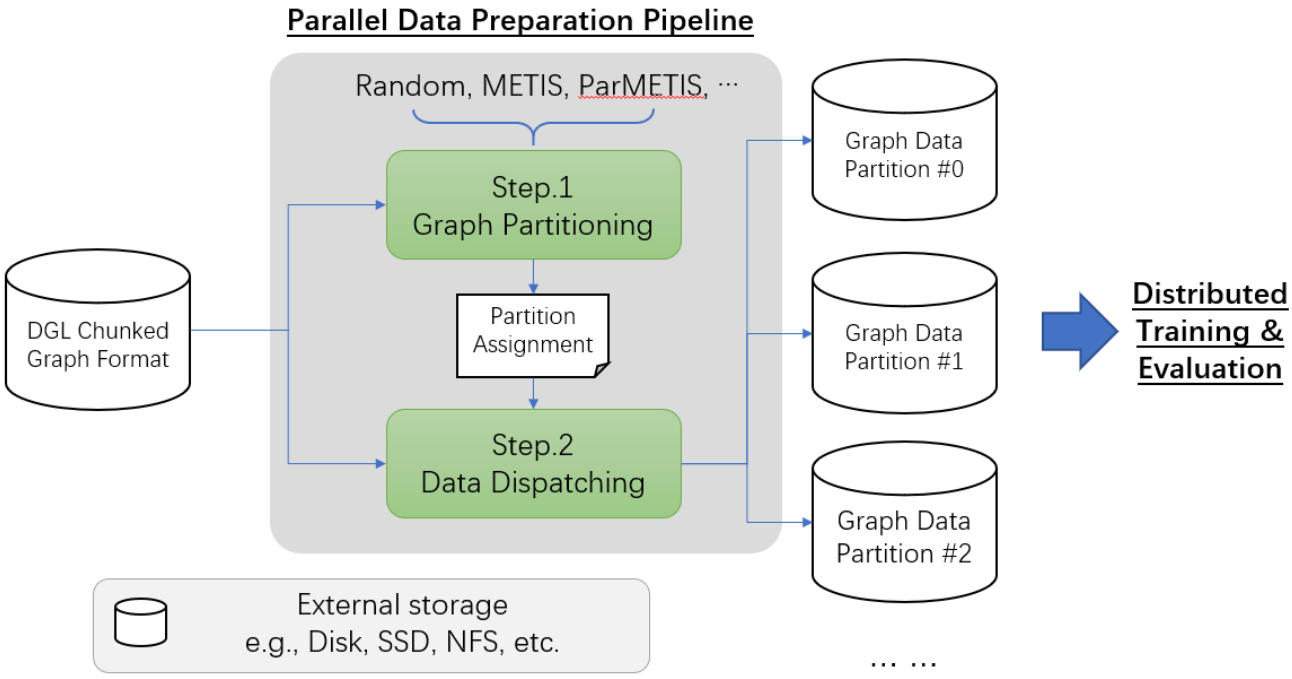
```
>>> import dgl
>>> # load partition 0
>>> part_data = dgl.distributed.load_partition('data_root_dir/graph_name.json', 0)
>>> g, nfeat, efeat, partition_book, graph_name, ntypes, etypes = part_data  # unpack
>>> print(g)
Graph(num_nodes=966043, num_edges=34270118,
      ndata_schemes={'orig_id': Scheme(shape=(), dtype=torch.int64),
                     'part_id': Scheme(shape=(), dtype=torch.int64),
                     '_ID': Scheme(shape=(), dtype=torch.int64),
                     'inner_node': Scheme(shape=(), dtype=torch.int32)}
      edata_schemes={'_ID': Scheme(shape=(), dtype=torch.int64),
                     'inner_edge': Scheme(shape=(), dtype=torch.int8),
                     'orig_id': Scheme(shape=(), dtype=torch.int64)})
```

As mentioned in the ID mapping section, each partition carries auxiliary information saved as ndata or edata such as original node/edge IDs, partition IDs, etc. Each partition not only saves nodes/edges it owns, but also includes node/edges that are adjacent to the partition (called **HALO** nodes/edges). The `inner_node` and `inner_edge` indicate whether a node/edge truely belongs to the partition (value is `True`) or is a HALO node/edge (value is `False`).

The `load_partition()` function loads all data at once. Users can load features or the partition book using the `dgl.distributed.load_partition_feats()` and `dgl.distributed.load_partition_book()` APIs respectively.

7.1.2 Distributed Graph Partitioning Pipeline

To handle massive graph data that cannot fit in the CPU RAM of a single machine, DGL utilizes data chunking and parallel processing to reduce memory footprint and running time. The figure below illustrates the pipeline:



- The pipeline takes input data stored in *Chunked Graph Format* and produces and dispatches data partitions to the target machines.
- **Step.1 Graph Partitioning:** It calculates the ownership of each partition and saves the results as a set of files called *partition assignment*. To speedup the step, some algorithms (e.g., ParMETIS) support parallel computing using multiple machines.
- **Step.2 Data Dispatching:** Given the partition assignment, the step then physically partitions the graph data and dispatches them to the machines user specified. It also converts the graph data into formats that are suitable for distributed training and evaluation.

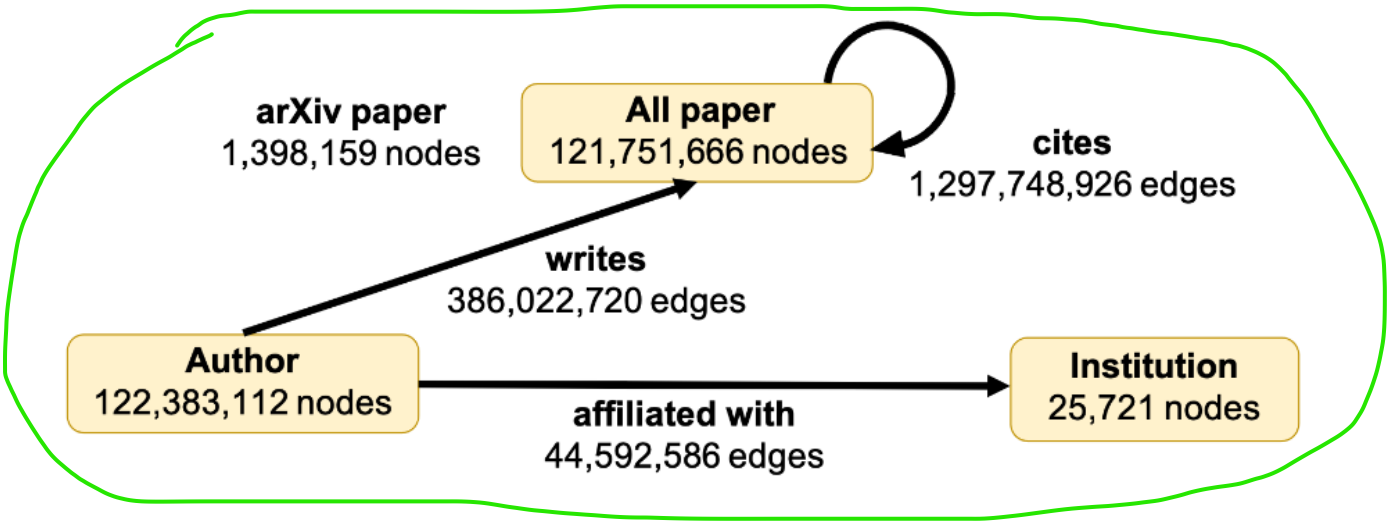
The whole pipeline is modularized so that each step can be invoked individually. For example, users can replace Step.1 with some custom graph partition algorithm as long as it produces partition assignment files correctly.

Chunked Graph Format

To run the pipeline, DGL requires the input graph to be stored in multiple data chunks. Each data chunk is the unit of data preprocessing and thus should fit into CPU RAM. In this section, we use the MAG240M-LSC data from Open Graph Benchmark as an example to describe the overall design, followed by a formal specification and tips for creating data in such format.

Example: MAG240M-LSC

The MAG240M-LSC graph is a heterogeneous academic graph extracted from the Microsoft Academic Graph (MAG), whose schema diagram is illustrated below:



Its raw data files are organized as follows:

```
/mydata/MAG240M-LSC/
  |-- meta.pt   # # A dictionary of the number of nodes for each type saved by torch.save,
  |             # as well as num_classes
  |-- processed/
    |-- author___affiliated_with___institution/
    |  |-- edge_index.npy            # graph, 713 MB
    |
    |-- paper/
    |  |-- node_feat.npy             # feature, 187 GB, (numpy memmap format)
    |  |-- node_label.npy            # label, 974 MB
    |  |-- node_year.npy             # year, 974 MB
    |
    |-- paper___cites___paper/
    |  |-- edge_index.npy            # graph, 21 GB
    |
    |-- author___writes___paper/
       |-- edge_index.npy            # graph, 6GB
```

The graph has three node types (`"paper"` , `"author"` and `"institution"`), three edge types/relations (`"cites"` , `"writes"` and `"affiliated_with"`). The `"paper"` nodes have three attributes (`"feat"` , `"label"` , `"year"`), while other types of nodes and edges are featureless. Below shows the data files when it is stored in DGL Chunked Graph Format:

```
/mydata/MAG240M-LSC_chunked/
  |-- metadata.json            # metadata json file
  |-- edges/                   # stores edge ID data
  |  |-- writes-part1.csv
  |  |-- writes-part2.csv
  |  |-- affiliated_with-part1.csv
  |  |-- affiliated_with-part2.csv
  |  |-- cites-part1.csv
  |  |-- cites-part1.csv
  |
  |-- node_data/               # stores node feature data
     |-- paper-feat-part1.npy
     |-- paper-feat-part2.npy
     |-- paper-label-part1.npy
     |-- paper-label-part2.npy
     |-- paper-year-part1.npy
     |-- paper-year-part2.npy
```

All the data files are chunked into two parts, including the edges of each relation (e.g., writes, affiliates, cites) and node features. If the graph has edge features, they will be chunked into multiple files too. All ID data are stored in CSV (we will illustrate the contents soon) while node features are stored in numpy arrays.

The `metadata.json` stores all the metadata information such as file names and chunk sizes (e.g., number of nodes, number of edges).

```
{
   "graph_name" : "MAG240M-LSC",  # given graph name
   "node_type": ["author", "paper", "institution"],
   "num_nodes_per_chunk": [
       [61191556, 61191556],      # number of author nodes per chunk
       [61191553, 61191552],      # number of paper nodes per chunk
       [12861, 12860]             # number of institution nodes per chunk
   ],
   # The edge type name is a colon-joined string of source, edge, and destination type.
   "edge_type": [
       "author:writes:paper",
       "author:affiliated_with:institution",
       "paper:cites:paper"
   ],
   "num_edges_per_chunk": [
       [193011360, 193011360],    # number of author:writes:paper edges per chunk
       [22296293, 22296293],      # number of author:affiliated_with:institution edges per
chunk
       [648874463, 648874463]     # number of paper:cites:paper edges per chunk
   ],
   "edges" : {
        "author:writes:paper" : {  # edge type
            "format" : {"name": "csv", "delimiter": " "},
            # The list of paths. Can be relative or absolute.
            "data" : ["edges/writes-part1.csv", "edges/writes-part2.csv"]
        },
        "author:affiliated_with:institution" : {
            "format" : {"name": "csv", "delimiter": " "},
            "data" : ["edges/affiliated_with-part1.csv", "edges/affiliated_with-part2.csv"]
        },
        "paper:cites:paper" : {
            "format" : {"name": "csv", "delimiter": " "},
            "data" : ["edges/cites-part1.csv", "edges/cites-part2.csv"]
        }
   },
   "node_data" : {
        "paper": {       # node type
            "feat": {   # feature key
                "format": {"name": "numpy"},
                "data": ["node_data/paper-feat-part1.npy", "node_data/paper-feat-part2.npy"]
            },
            "label": {   # feature key
                "format": {"name": "numpy"},
                "data": ["node_data/paper-label-part1.npy", "node_data/paper-label-part2.npy"]
            },
            "year": {   # feature key
                "format": {"name": "numpy"},
                "data": ["node_data/paper-year-part1.npy", "node_data/paper-year-part2.npy"]
            }
        }
   },
   "edge_data" : {}  # MAG240M-LSC does not have edge features
}
```

There are three parts in `metadata.json`:

- Graph schema information and chunk sizes, e.g., `"node_type"` , `"num_nodes_per_chunk"`, etc.
- Edge index data under key `"edges"`.
- Node/edge feature data under keys `"node_data"` and `"edge_data"`.

The edge index files contain edges in the form of node ID pairs:

```
# writes-part1.csv
0 0
0 1
0 20
0 29
0 1203
...
```

Specification

In general, a chunked graph data folder just needs a `metadata.json` and a bunch of data files. The folder structure in the MAG240M-LSC example is not a strict requirement as long as `metadata.json` contains valid file paths.

`metadata.json` top-level keys:

- `graph_name`: String. Unique name used by `dgl.distributed.DistGraph` to load graph.
- `node_type`: List of string. Node type names.
- `num_nodes_per_chunk`: List of list of integer. For graphs with T node types stored in P chunks, the value contains T integer lists. Each list contains P integers, which specify the number of nodes in each chunk.
- `edge_type`: List of string. Edge type names in the form of `<source node type>:<relation>:<destination node type>`.
- `num_edges_per_chunk`: List of list of integer. For graphs with R edge types stored in P chunks, the value contains R integer lists. Each list contains P integers, which specify the number of edges in each chunk.
- `edges`: Dict of `ChunkFileSpec`. Edge index files. Dictionary keys are edge type names in the form of `<source node type>:<relation>:<destination node type>`.
- `node_data`: Dict of `ChunkFileSpec`. Data files that store node attributes could have arbitrary number of files regardless of `num_parts`. Dictionary keys are node type names.
- `edge_data`: Dict of `ChunkFileSpec`. Data files that store edge attributes could have arbitrary number of files regardless of `num_parts`. Dictionary keys are edge type names in the form of `<source node type>:<relation>:<destination node type>`.

`ChunkFileSpec` has two keys:

- `format`: File format. Depending on the format `name`, users can configure more details about how to parse each data file.
    - `"csv"`: CSV file. Use the `delimiter` key to specify delimiter in use.
    - `"numpy"`: NumPy array binary file created by `numpy.save()`.
    - `"parquet"`: parquet table binary file created by `pyarrow.parquet.write_table()`.
- `data`: List of string. File path to each data chunk. Support absolute path.

Tips for making chunked graph data

Depending on the raw data, the implementation could include:

- Construct graphs out of non-structured data such as texts or tabular data.
- Augment or transform the input graph struture or features. E.g., adding reverse or self-loop edges, normalizing features, etc.
- Chunk the input graph structure and features into multiple data files so that each one can fit in CPU RAM for subsequent preprocessing steps.

To avoid running into out-of-memory error, it is recommended to process graph structures and feature data separately. Processing one chunk at a time can also reduce the maximal runtime memory footprint. As an example, DGL provides a tools/chunk_graph.py script that chunks an in-memory feature-less `DGLGraph` and feature tensors stored in `numpy.memmap`.

Step.1 Graph Partitioning

This step reads the chunked graph data and calculates which partition each node should belong to. The results are saved in a set of *partition assignment files*. For example, to randomly partition MAG240M-LSC to two parts, run the `partition_algo/random_partition.py` script in the `tools` folder:

```
python /my/repo/dgl/tools/partition_algo/random_partition.py
    --in_dir /mydata/MAG240M-LSC_chunked
    --out_dir /mydata/MAG240M-LSC_2parts
    --num_partitions 2
```

, which outputs files as follows:

```
MAG240M-LSC_2parts/
  |-- paper.txt
  |-- author.txt
  |-- institution.txt
```

Each file stores the partition assignment of the corresponding node type. The contents are the partition ID of each node stored in lines, i.e., line i is the partition ID of node i.

```
# paper.txt
0
1
1
0
0
1
0
...
```

Despite its simplicity, random partitioning may result in frequent cross-machine communication. Check out chapter 7.4 Advanced Graph Partitioning for more advanced options.

Step.2 Data Dispatching

DGL provides a `dispatch_data.py` script to physically partition the data and dispatch partitions to each training machines. It will also convert the data once again to data objects that can be loaded by DGL training processes efficiently. The entire step can be further accelerated using multi-processing.

```
python /myrepo/dgl/tools/dispatch_data.py          \
   --in-dir /mydata/MAG240M-LSC_chunked/           \
   --partitions-dir /mydata/MAG240M-LSC_2parts/    \
   --out-dir data/MAG_LSC_partitioned              \
   --ip-config ip_config.txt
```

- `--in-dir` specifies the path to the folder of the input chunked graph data produced
- `--partitions-dir` specifies the path to the partition assignment folder produced by Step.1.
- `--out-dir` specifies the path to stored the data partition on each machine.
- `--ip-config` specifies the IP configuration file of the cluster.

An example IP configuration file is as follows:

```
172.31.19.1
172.31.23.205
```

As a counterpart of `return_mapping=True` in `partition_graph()`, the distributed partitioning pipeline provides two arguments in `dispatch_data.py` to save the original node/edge IDs to disk.

- `--save-orig-nids` save original node IDs into files.
- `--save-orig-eids` save original edge IDs into files.

Specifying the two options will create two files `orig_nids.dgl` and `orig_eids.dgl` under each partition folder.

```
data_root_dir/
  |-- graph_name.json       # partition configuration file in JSON
  |-- part0/                # data for partition 0
  |  |-- orig_nids.dgl      # original node IDs
  |  |-- orig_eids.dgl      # original edge IDs
  |  |-- ...                # other data such as graph and node/edge feats
  |
  |-- part1/                # data for partition 1
  |  |-- orig_nids.dgl
  |  |-- orig_eids.dgl
  |  |-- ...
  |
  |-- ...                   # data for other partitions
```

The two files store the original IDs as a dictionary of tensors, where keys are node/edge type names and values are ID tensors. Users can use the `dgl.data.load_tensors()` utility to load them:

```
# Load the original IDs for the nodes in partition 0.
orig_nids_0 = dgl.data.load_tensors('/path/to/data/part0/orig_nids.dgl')
# Get the original node IDs for node type 'user'
user_orig_nids_0 = orig_nids_0['user']

# Load the original IDs for the edges in partition 0.
orig_eids_0 = dgl.data.load_tensors('/path/to/data/part0/orig_eids.dgl')
# Get the original edge IDs for edge type 'like'
like_orig_eids_0 = orig_nids_0['like']
```

During data dispatching, DGL assumes that the combined CPU RAM of the cluster is able to hold the entire graph data. Node ownership is determined by the result of partitioning algorithm where as for edges the owner of the destination node also owns the edge as well.