SPRACE

DGL Study part I

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SPRACE-ML (track-ml)

Deep Graph Library (DGL)

DGL is a Python package built for implementation of graph neural network model family, on top of existing DL frameworks (e.g. PyTorch, MXNet, Gluon etc.).

DGL provides:

- Versatile controls over **message passing**
- Transparent **speed optimization** with automatic batching of computations and s**parse matrix multiplication**
- Good scalability to graphs with **tens of millions of vertices**

Installation (DGL)

With conda installed, you will want install DGL into Python 3.5 conda environment.

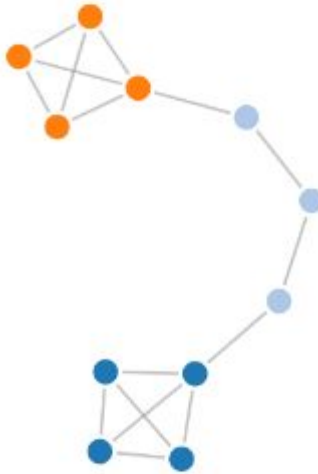
After the conda environment is activated, run one of the following commands to fit with your cuda version:

```
conda install -c dglteam dgl                # For CPU Build
conda install -c dglteam dgl-cuda9.0        # For CUDA 9.0 Build
conda install -c dglteam dgl-cuda10.0       # For CUDA 10.0 Build
conda install -c dglteam dgl-cuda10.1       # For CUDA 10.1 Build
conda install -c dglteam dgl-cuda10.2       # For CUDA 10.2 Build
```

NetworkX
Network Analysis in Python

NetworkX is a Python package for the creation, manipulation, and study of the structure, dynamics, and functions of complex networks.

- Data structures for graphs, digraphs, and multigraphs
- Many standard graph algorithms
- Network structure and analysis measures
- Generators for classic graphs, random graphs, and synthetic networks
- Nodes can be "anything" (e.g., text, images, XML records)
- Edges can hold arbitrary data (e.g., weights, time-series)

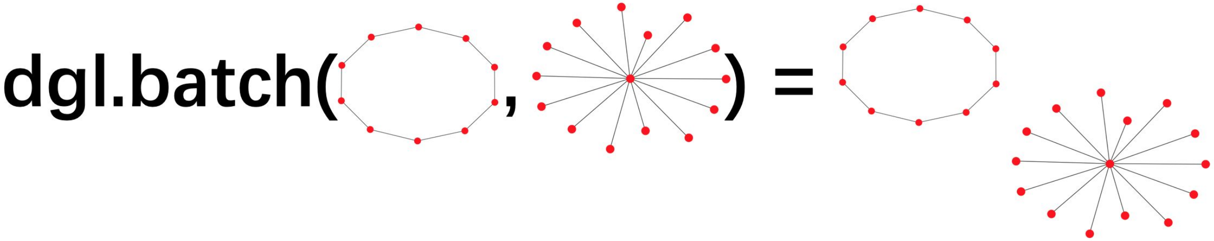


To install:

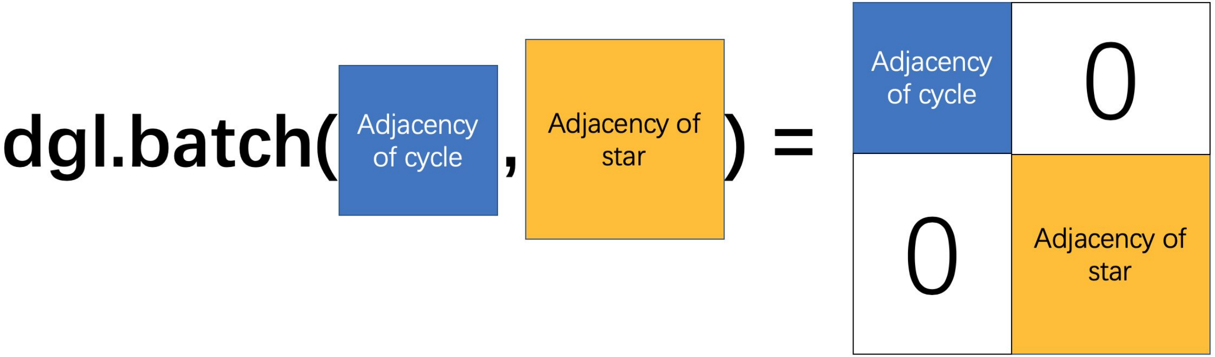
```
conda install networkx  # or
pip install networkx
```

Dataset

DGL has a dataset class called MiniGCDataset. this class can generate a dataset with eight different types of graphs and each class has the same number of graph samples.



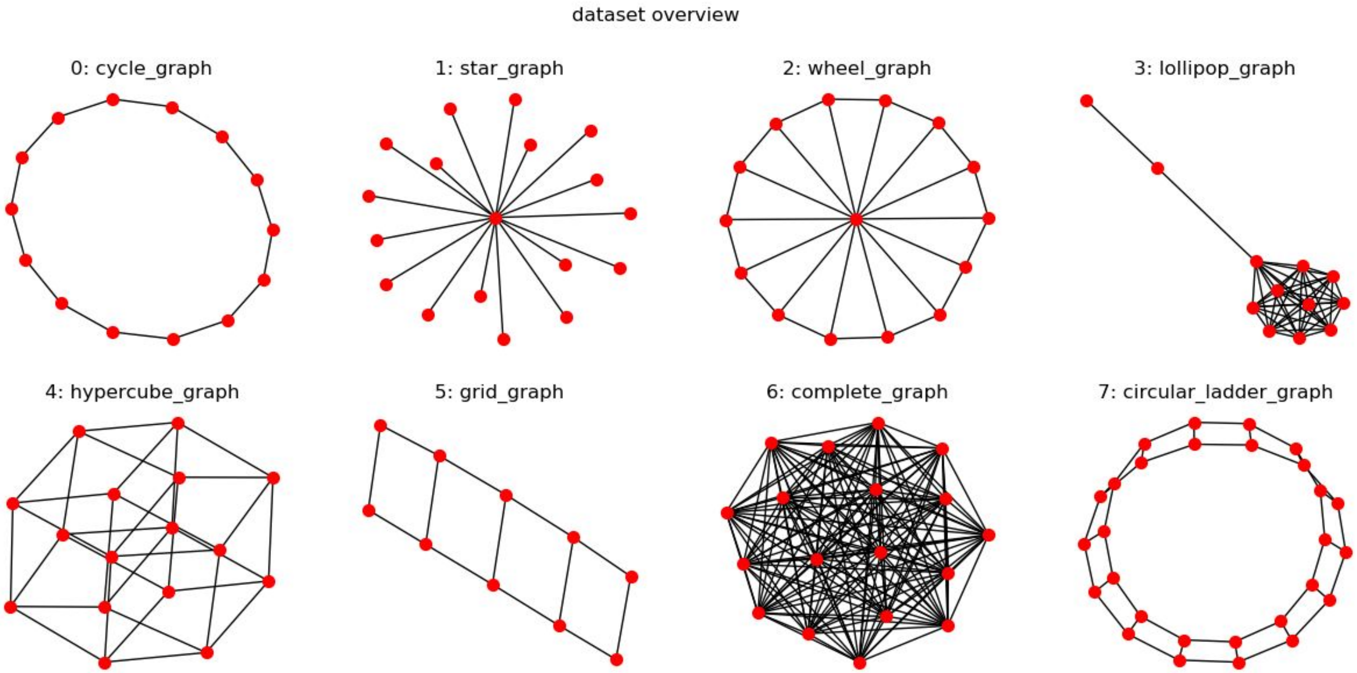
dgl.batch(,) =



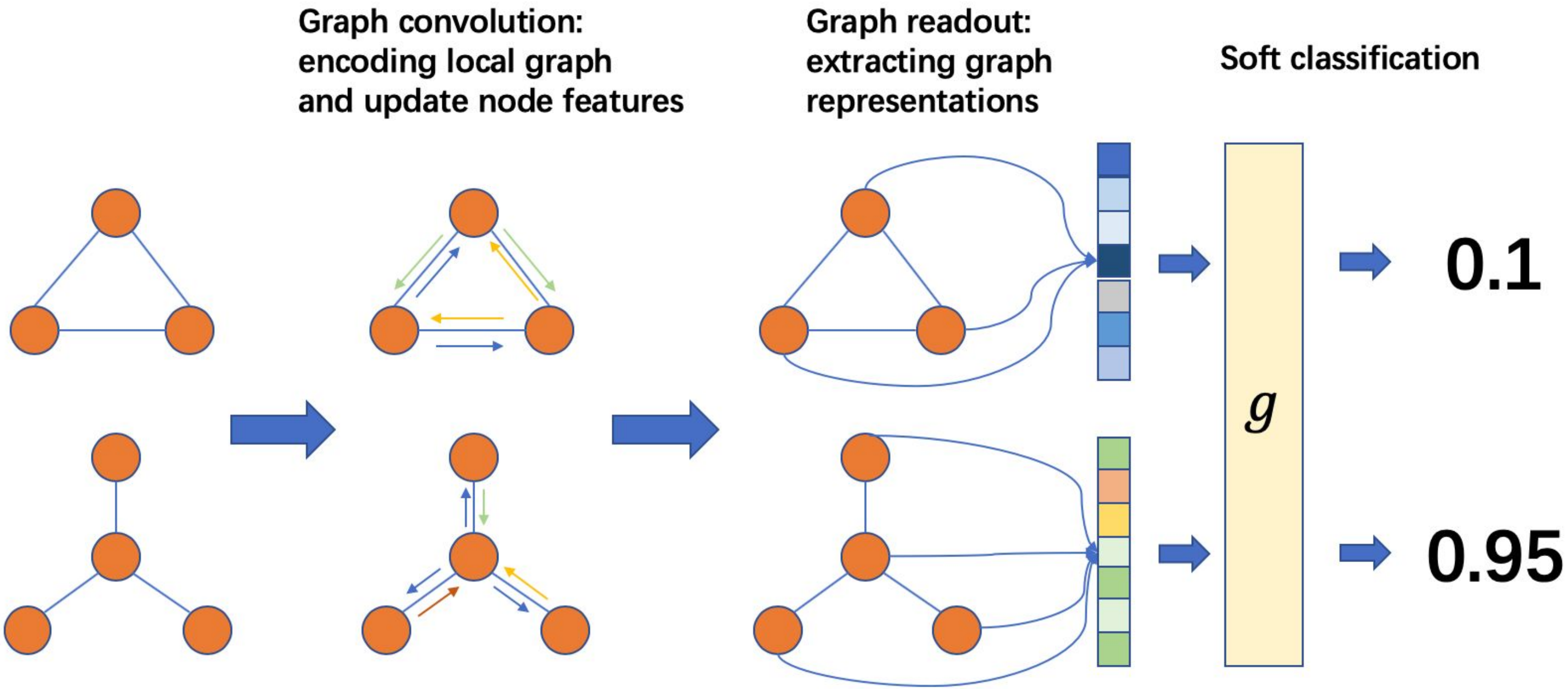
dgl.batch(Adjacency of cycle, Adjacency of star) =

Adjacency of cycle	0
0	Adjacency of star

Part I - Graph Classification



Classifier



Graph convolution: encoding local graph and update node features

Graph readout: extracting graph representations

Soft classification