dortmund university

Stanford University

PyG 2.0

Advanced Representation Learning on Graphs

Matthias Fey

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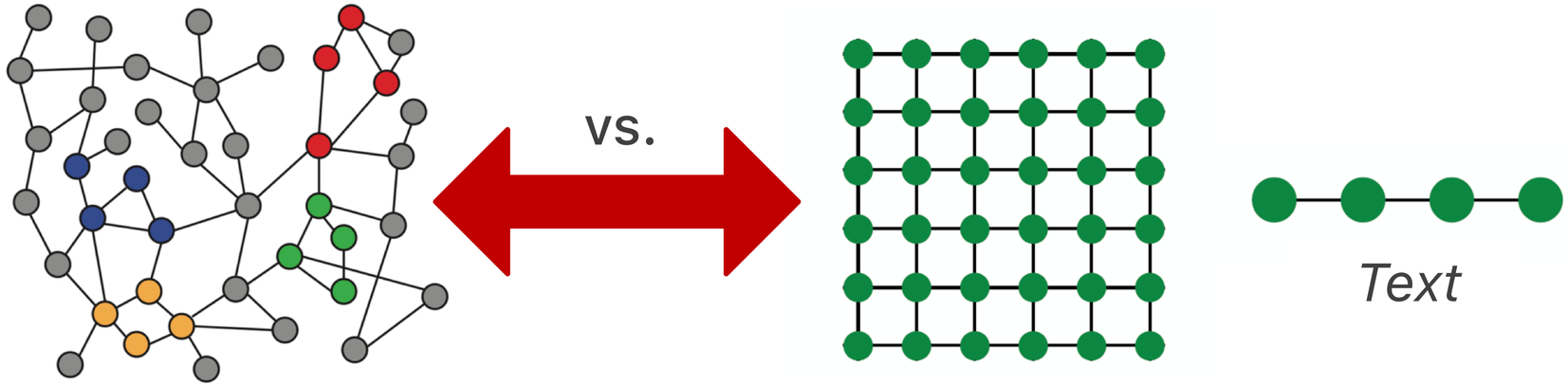
https://pyg.org

/pyg-team/pytorch-geometric


```
conda install pyg -c pyg
```

Motivation

The **modern deep learning toolbox** is designed for **sequences and grids**



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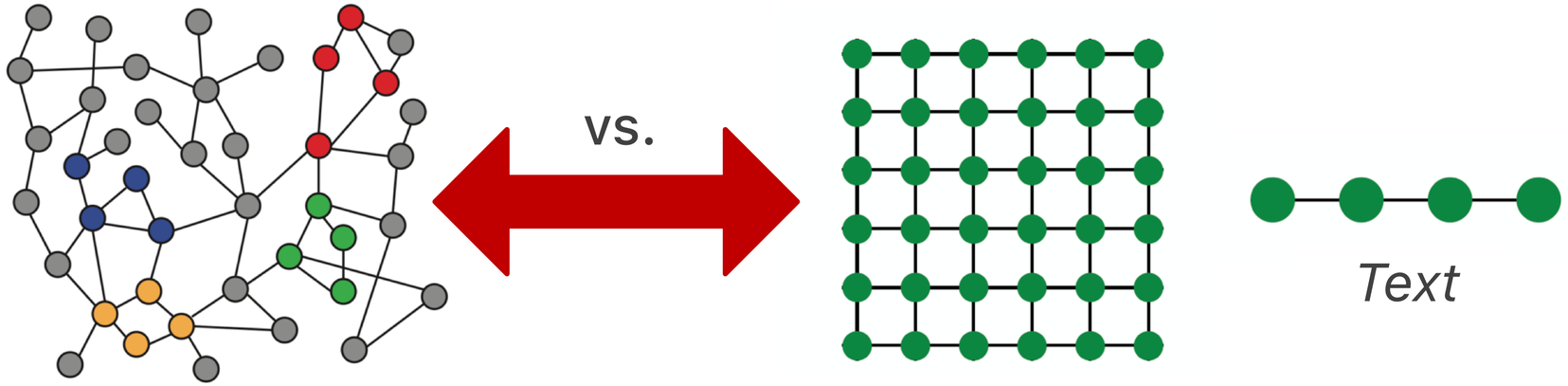

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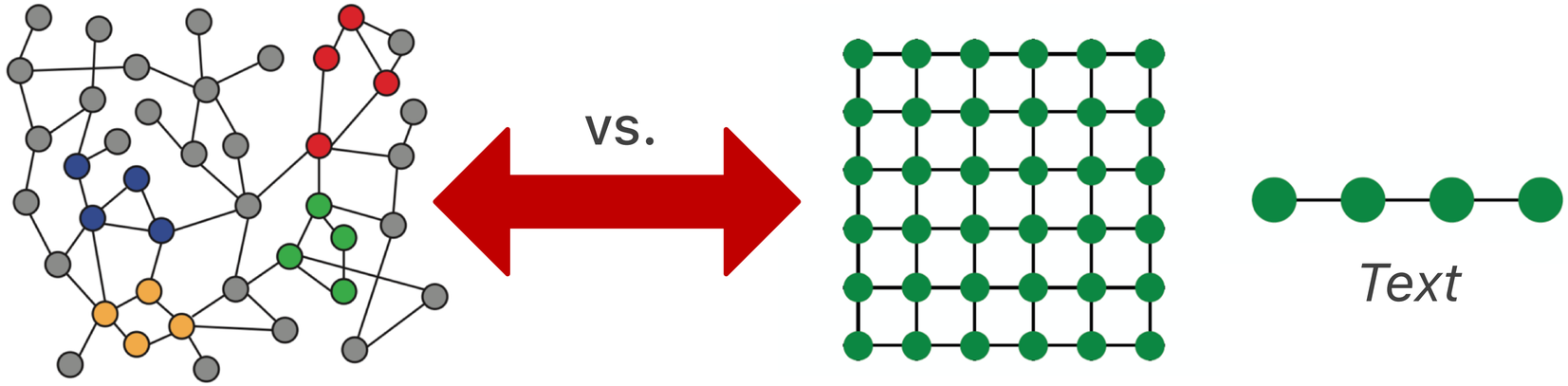

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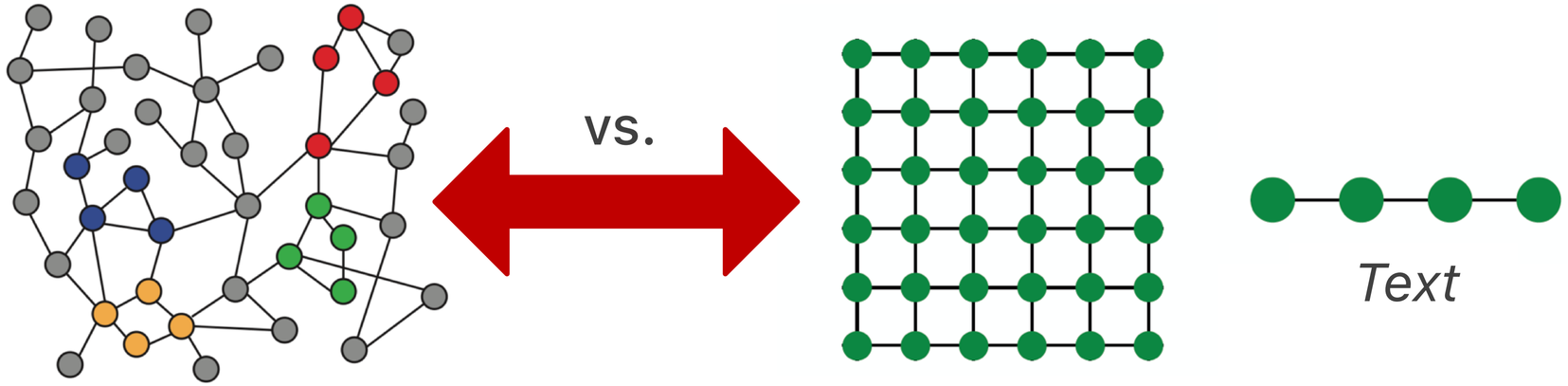

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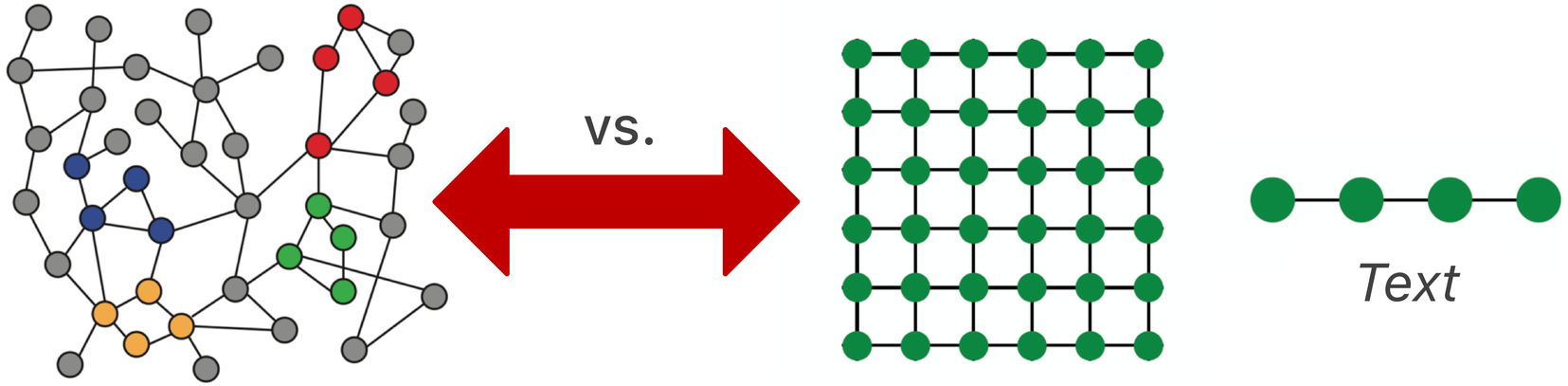

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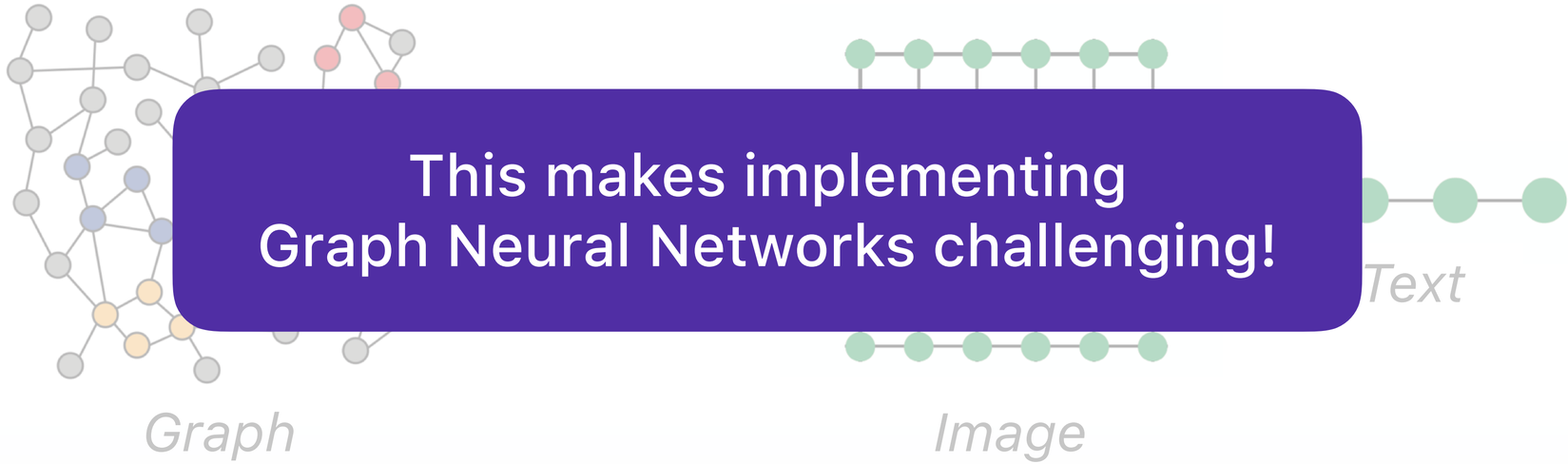

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- **PyG** fits nicely into the **PyTorch ecosystem**
  *Scaling up models via **PyTorch Lightning***
  *Explaining models via **Captum***

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```python
from torch.nn import Conv2d

class CNN(torch.nn.Module):
    def __init__(self):
        self.conv1 = Conv2d(3, 64)
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from torch_geometric.nn import GCNConv

class GNN(torch.nn.Module):
    def __init__(self):
        self.conv1 = GCNConv(3, 64)
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    def forward(self, input, edge_index):
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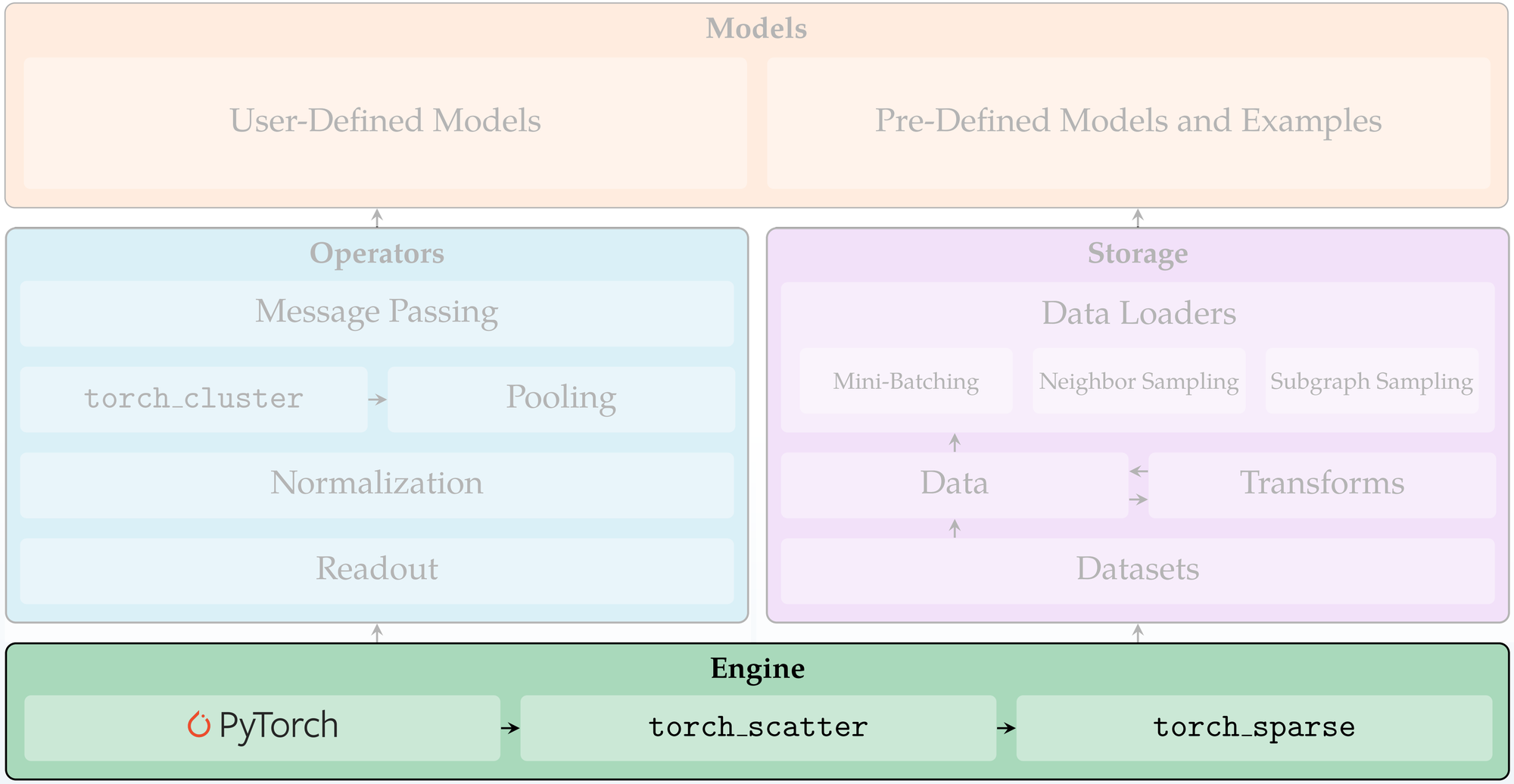

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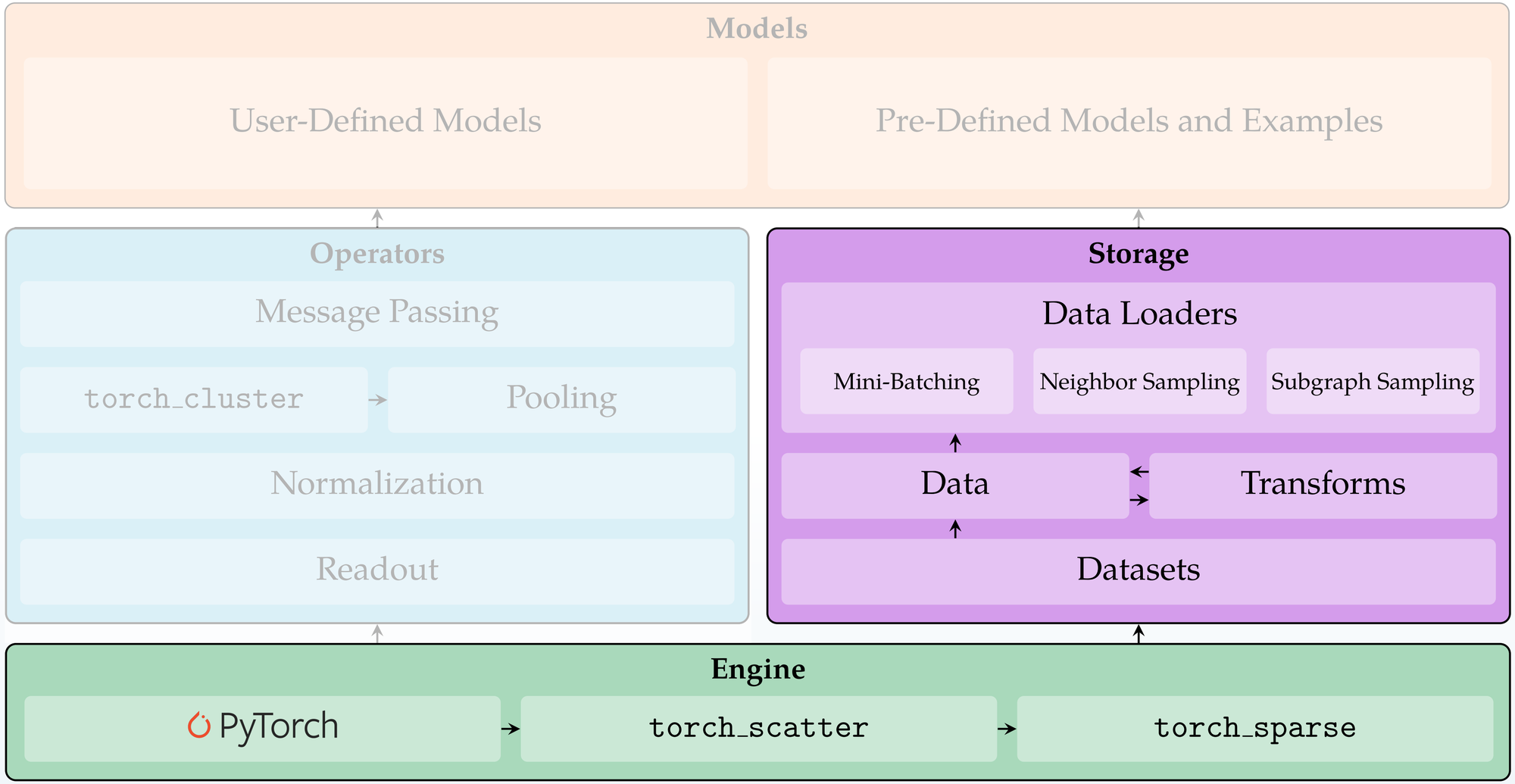

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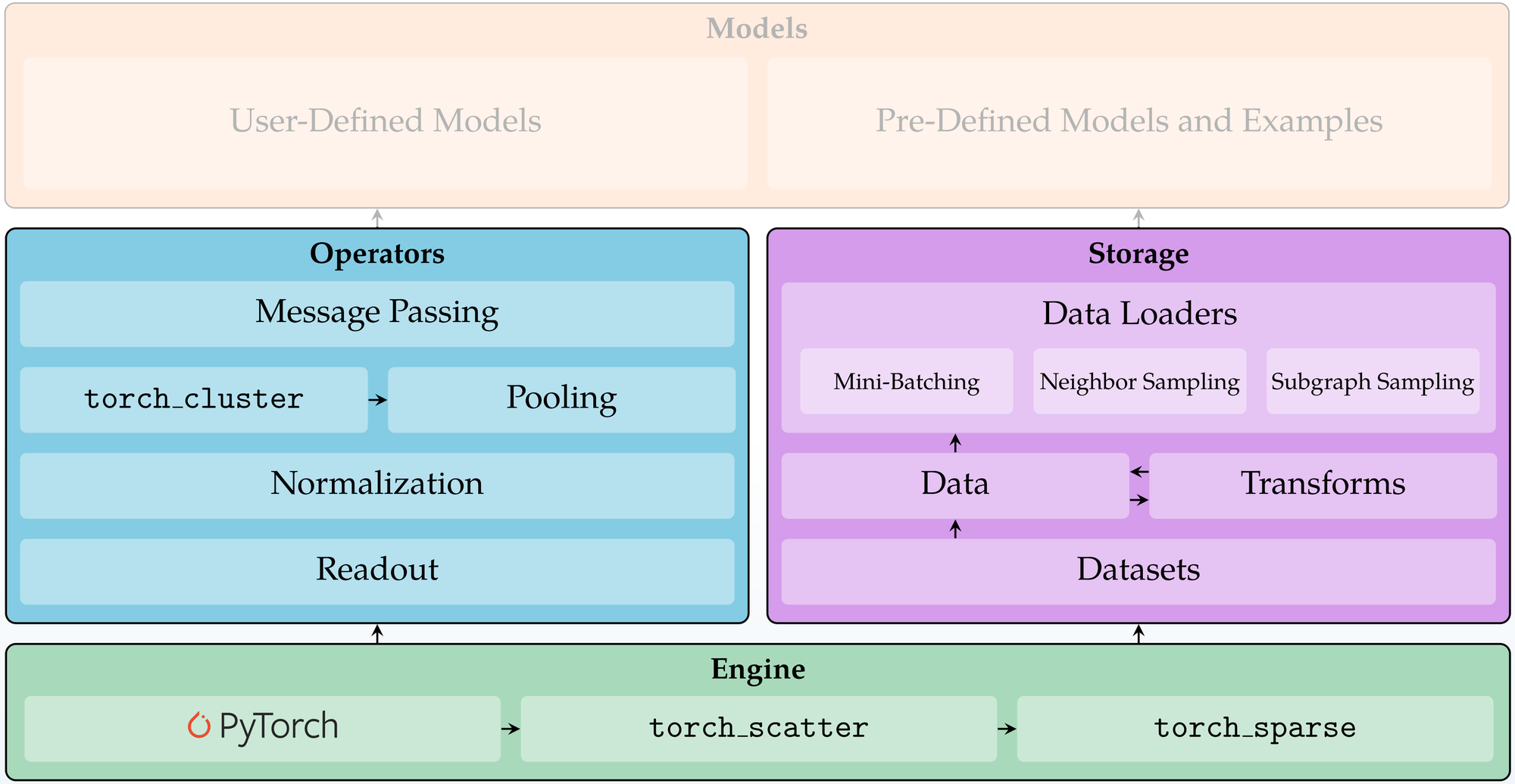

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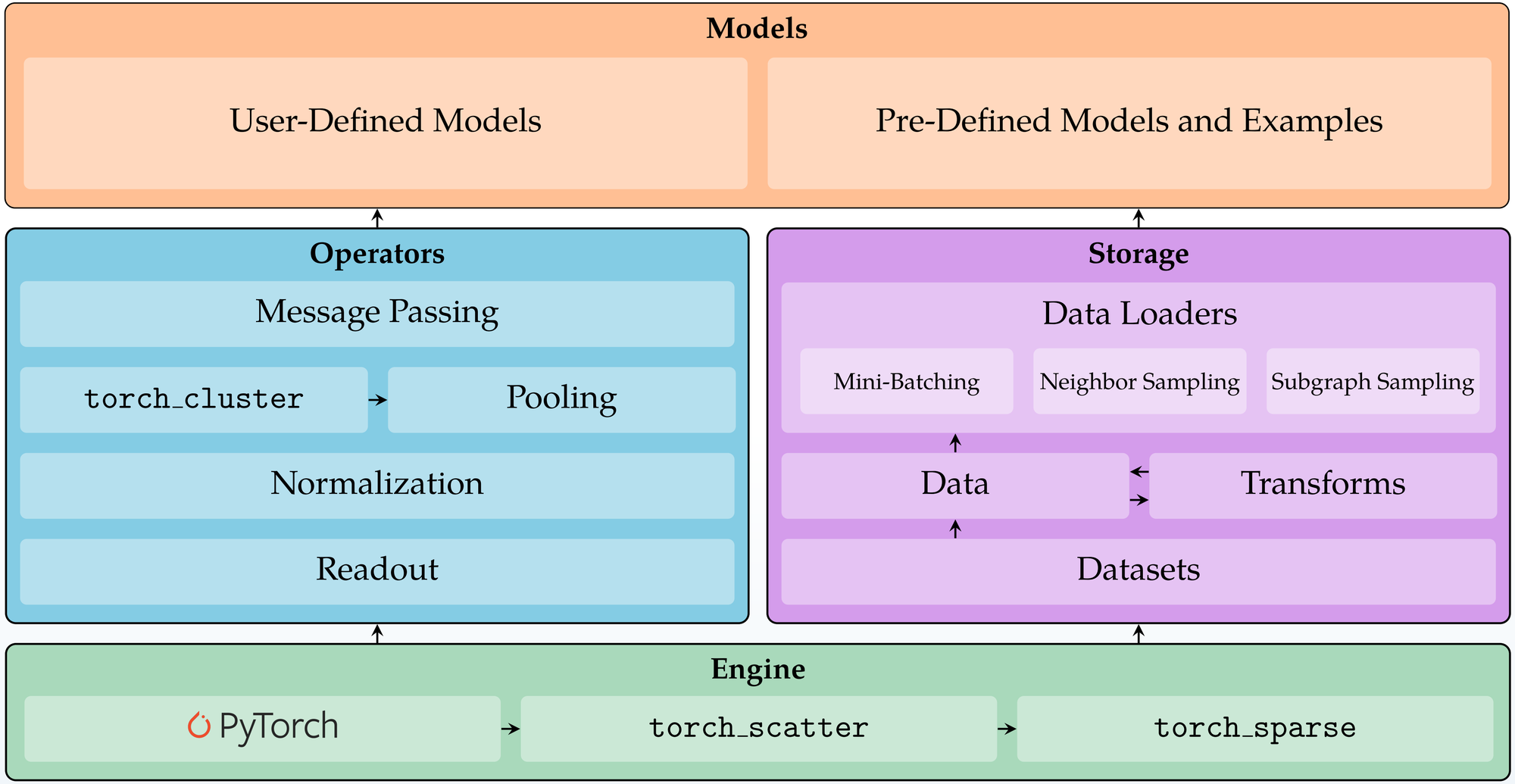
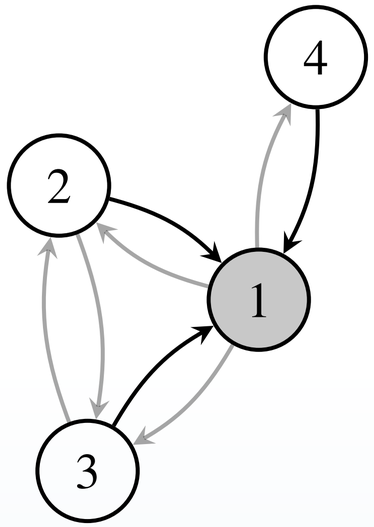


Message Passing Graph Neural Networks



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- input node features $\mathbf{H}^{(0)} \in \mathbb{R}^{|\mathcal{V}| \times C}$
- edge indices $\mathbf{I} \in \{1, ..., |\mathcal{V}|\}^{2 \times |\mathcal{E}|}$
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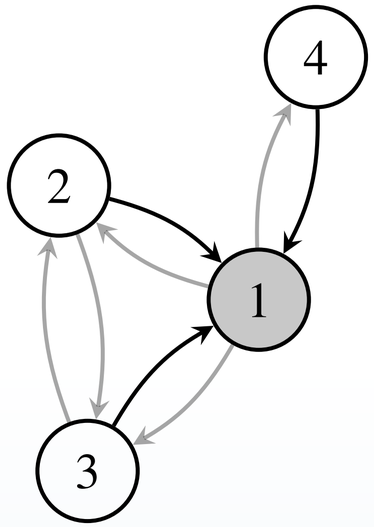

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Message Passing Scheme

permutation-invariant aggregation operator, e.g., *sum*, *mean* or *max*

$$\mathbf{h}_i^{(\ell+1)} = \textsc{Update}_\theta \left(\mathbf{h}_i^{(\ell)}, \bigoplus_{j \in \mathcal{N}(i)} \textsc{Message}_\theta \left(\mathbf{h}_j^{(\ell)}, \mathbf{h}_i^{(\ell)}, \mathbf{e}_{j,i} \right) \right)$$

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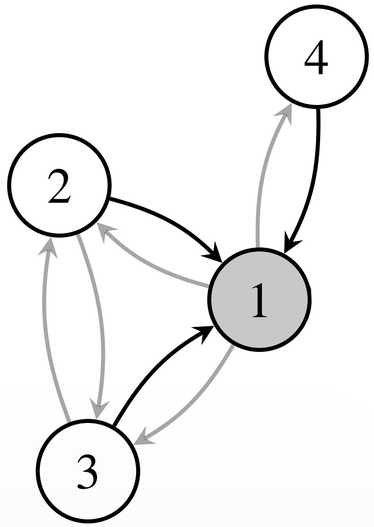
Flexible implementation via *parallelizable* `gather` and `scatter` operations condensed in a general `MessagePassing` interface



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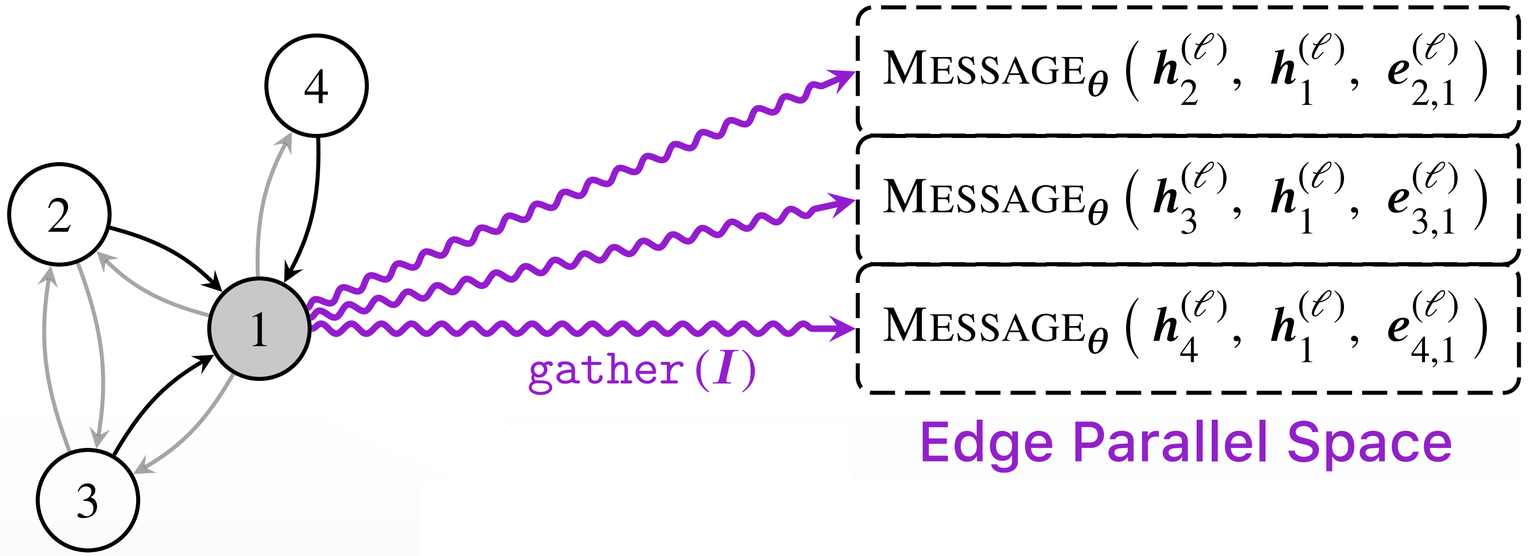

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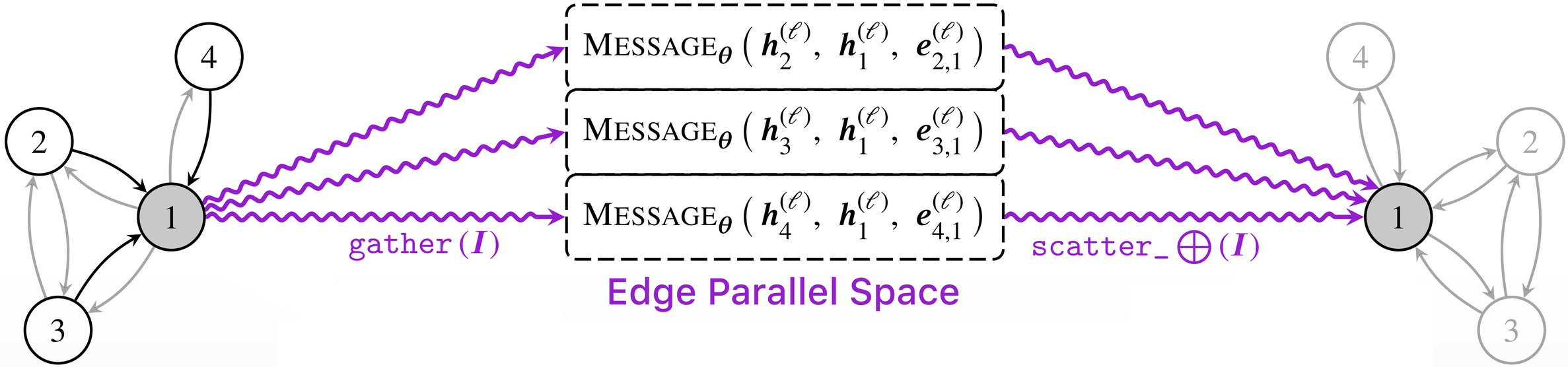

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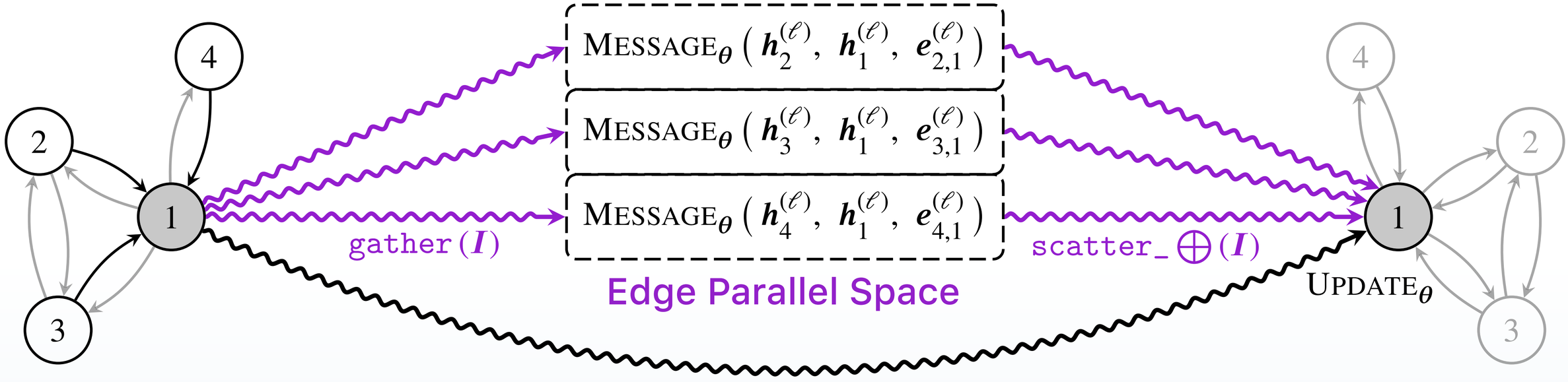

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GNN layers:

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GNN models:

GAE ARGA DGI Node2Vec Graph-UNet AFP C&S LP RECT
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Not all GNN operators need to **explicitly materialize** the edge parallel space

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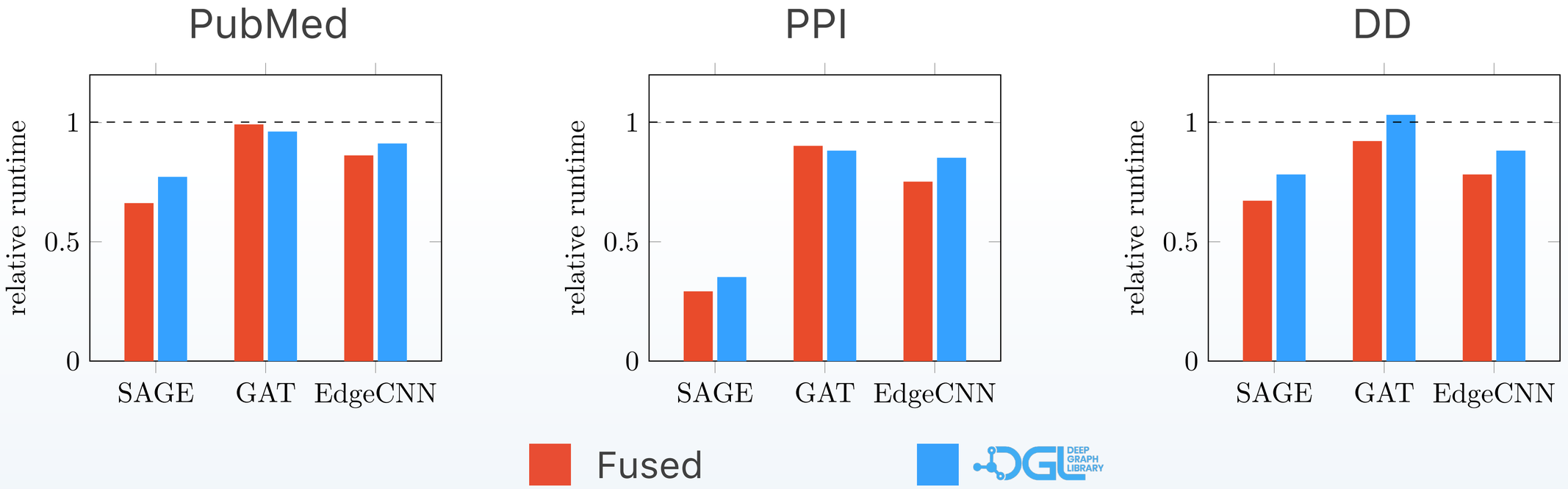

Mini-Batching in GNNs

PyG supports mini-batching on **many small graphs**

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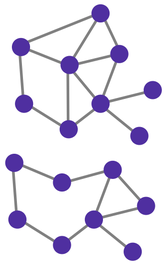

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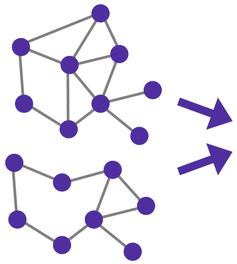

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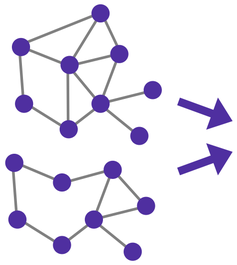

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from torch_geometric.datasets import TUDataset
from torch_geometric.loader import DataLoader

dataset = TUDataset(name='IMDB-BINARY')
loader = DataLoader(dataset, batch_size=128)
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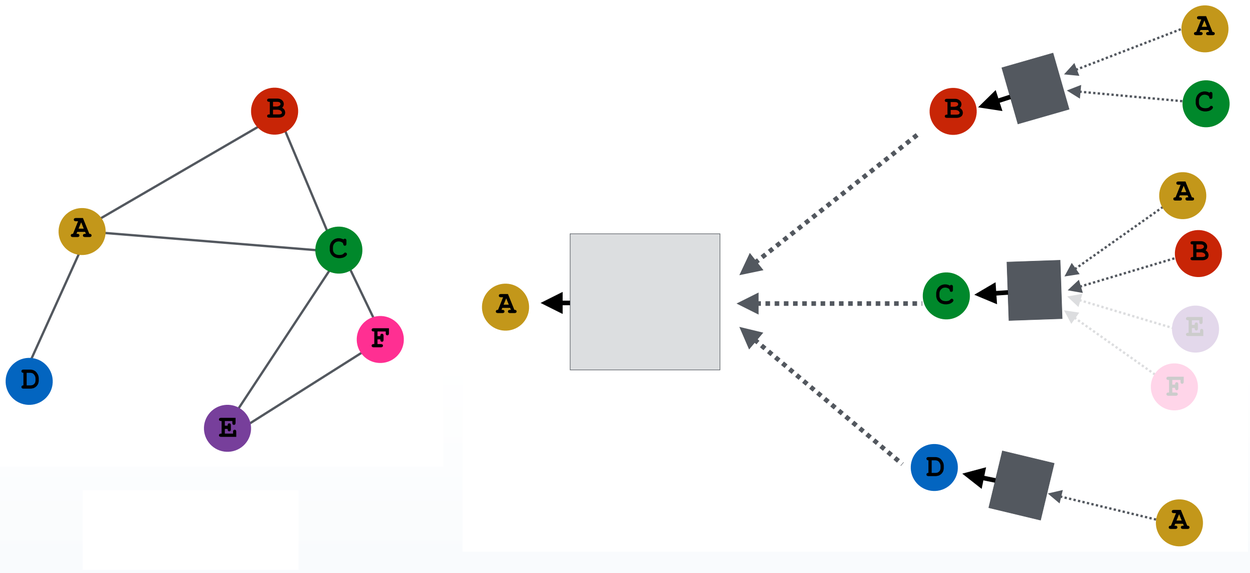

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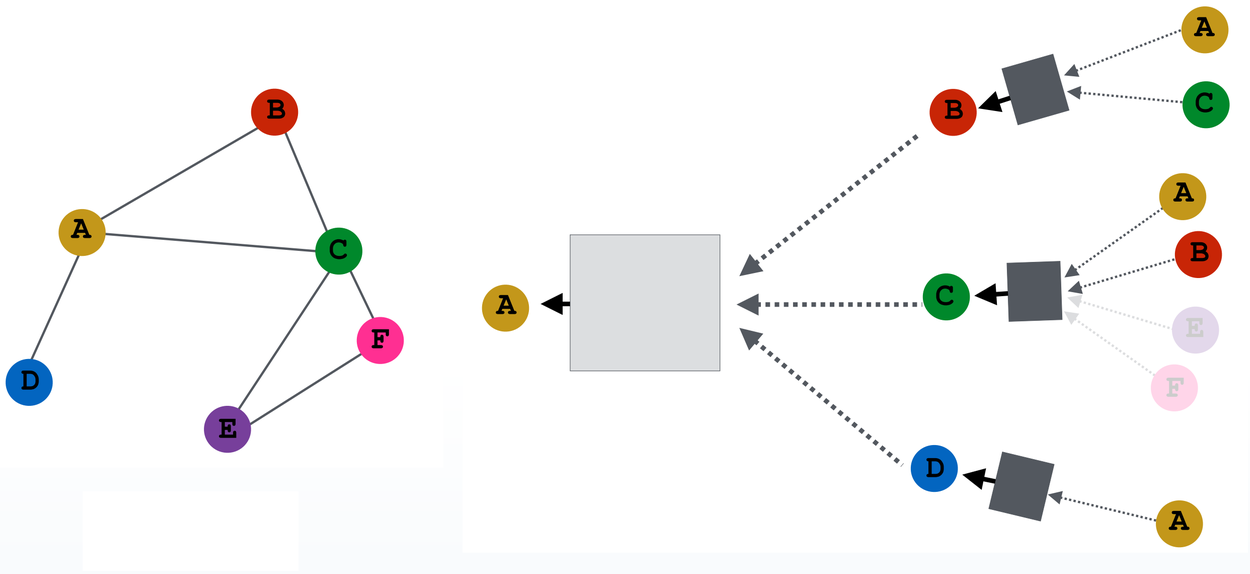


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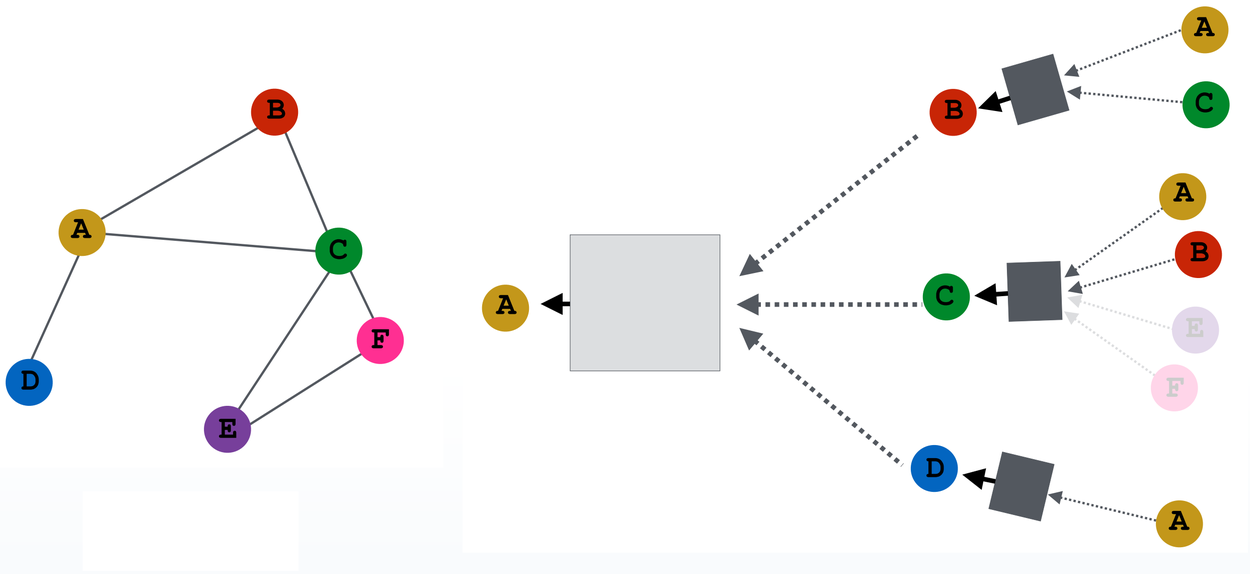


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Scalability support:

NeighborSampling ClusterGCN GraphSAINT ShaDow
SGC SIGN Correct&Smooth GNNAutoScale

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Predict the class of a node

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Unsupervised Learning Self-Supervised Learning
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Unsupervised Learning **Self-Supervised Learning**
Few/Zero-Shot Learning **Pre-Training** **Explainability** ...

PyG provides over **80 examples** with access to over **200 benchmark datasets** to get familiar with the **latest trends in graph machine learning**

Additional Features

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Convert pure Python GNN model to an **optimized** and **standalone** program

```
class GNN(torch.nn.Module):
    def __init__(self):
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Additional Features

TorchScript

Convert pure Python GNN model to an **optimized** and **standalone** program

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PyTorch Lightning

1. Choose a **GNN model**
2. Setup a **trainer**
   (#GPUs, accelerator type)
3. Call `trainer.fit()`

```python
data = Reddit('data/Reddit')
model = GraphSAGE(in_channels, out_channels)

trainer = Trainer(gpus=2, accelerator='ddp')

trainer.fit(model, data)
trainer.test()
```

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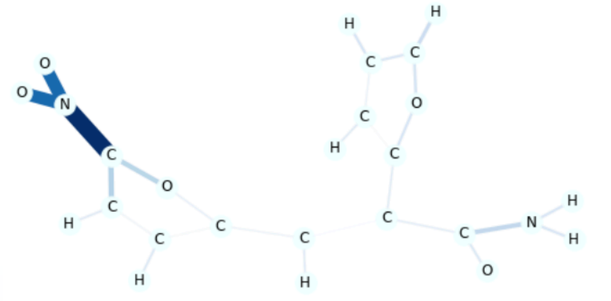
Captum

Explain GNN predictions out-of-the-box



```
from captum.attr import IntegratedGradients

ig = IntegratedGradients(model)
ig.attribute(input, edge_index, target=0)
```

Success Stories

- ~700 research papers using PyG
- ~2M weekly wheel downloads
- ~180 external contributors
- ~600 members on Slack

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@ylecun

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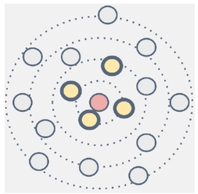
PyG already has its own ecosystem:

PyTorch Geometric Temporal

Dive into Graphs



DeepGCNs

Open Catalyst Project

FACEBOOK AI

Success Stories

OPEN GRAPH BENCHMARK

https://ogb.stanford.edu
/snap-stanford/ogb

- OGB provides a variety of **realistic** and **large-scale** graph benchmark datasets
- Data loaders are **compatible** with **PyG**
- Dive-in examples are **utilizing** **PyG**

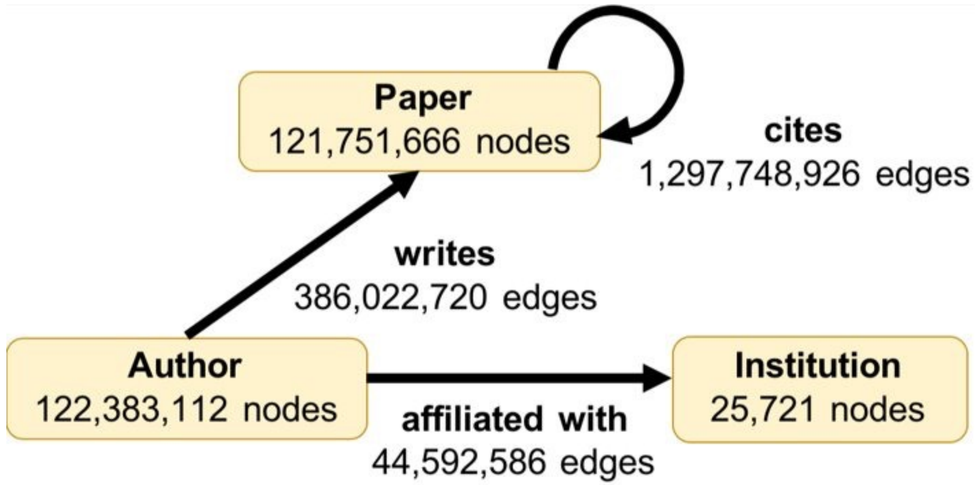
```python
from ogb import PygGraphPropPredDataset
from torch_geometric.loader import DataLoader

dataset = PygGraphPropPredDataset('ogbg-molhiv')
loader = DataLoader(dataset, batch_size=128)
```

Success Stories

OGB-LSC — Large-Scale Challenge @ KDD Cup 2021

Competition on **three large-scale graph datasets**, *e.g.*:



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- **~1.7B edges** across three edge types

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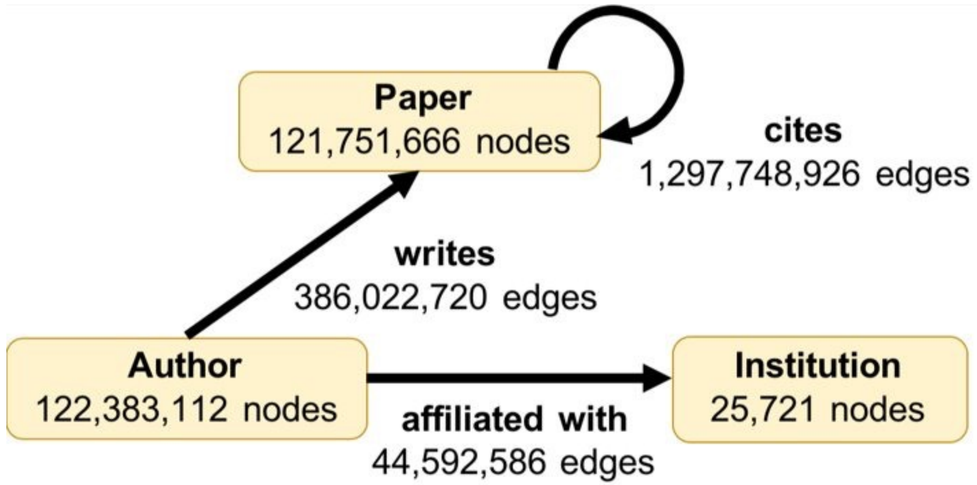

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We used PyG to benchmark GNNs:

Model	#Params	Validation	Test
MLP	0.5M	52.67	52.73
LabelProp	0	58.44	56.29
SGC	0.7M	65.82	65.29
SIGN	3.8M	66.64	66.09
MLP+C&S	0.5M	66.98	66.18
GraphSAGE (NS)	4.9M	66.79	66.28
GAT (NS)	4.9M	67.15	66.80
R-GraphSAGE (NS)	12.2M	69.86	68.94
R-GAT (NS)	12.3M	**70.02**	**69.42**

Joining Forces

We have build a **larger team** for the **future development** of **PyG**, in close collaboration with

dortmund university

Stanford University

https://pyg.org

- ensure **longevity** of **PyG**
- integrate tools from both parties into a **unified package**
- keep up with **integrating latest trends** in academic research
- extend **its scope** to better support real-world use-cases
- make it *(even)* **easier to use** for both academia and industry
- make it *(even)* **more scalable**

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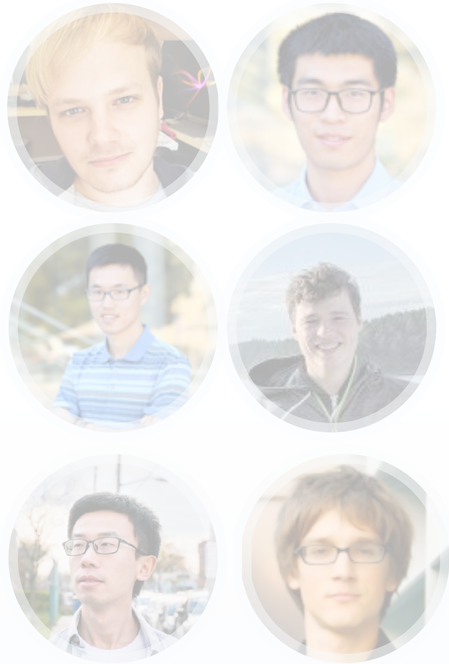

dortmund university

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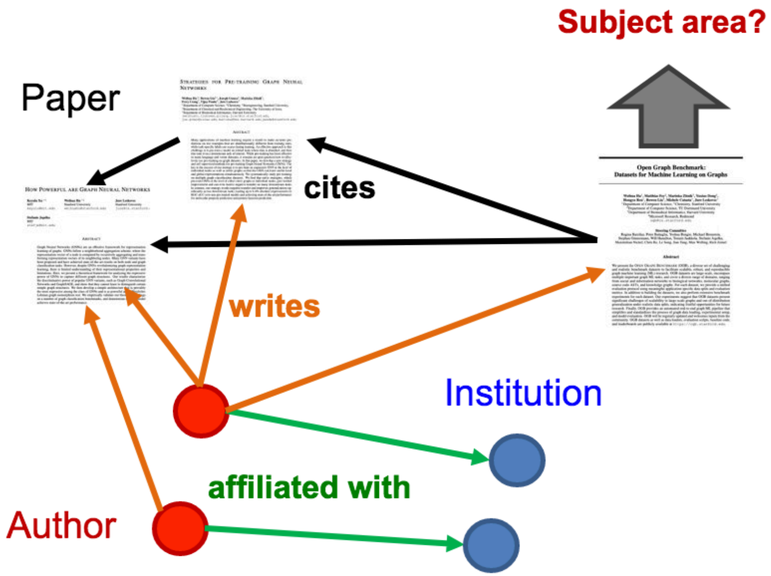
PyG 2.0

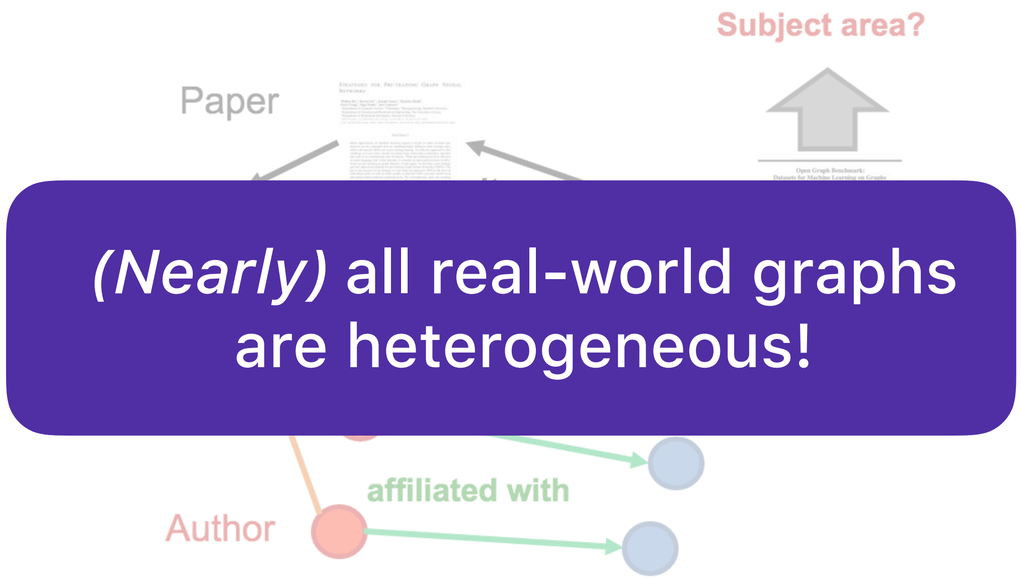
Advanced Representation Learning on Graphs

Overview



Heterogeneous Graphs

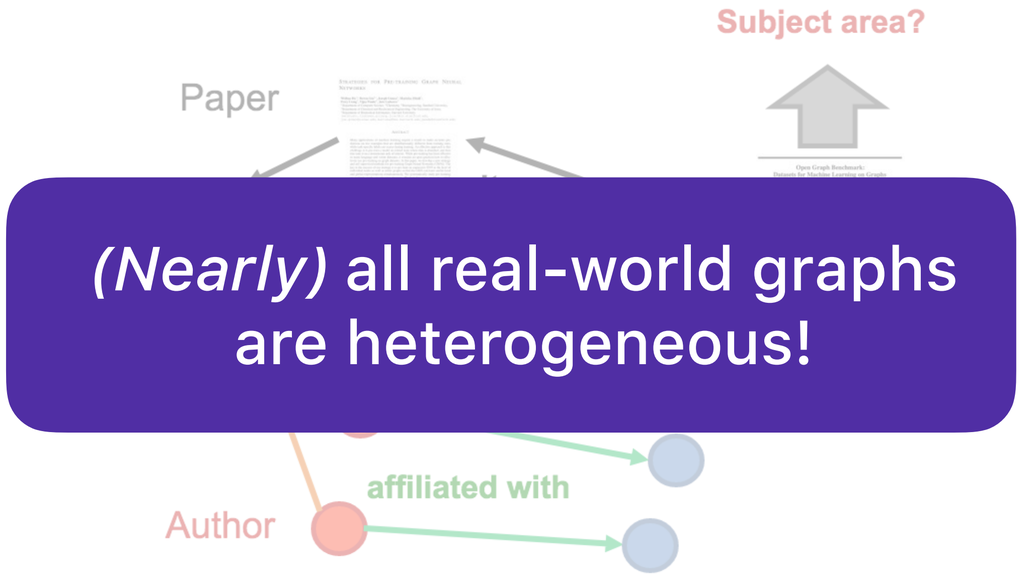
Overview



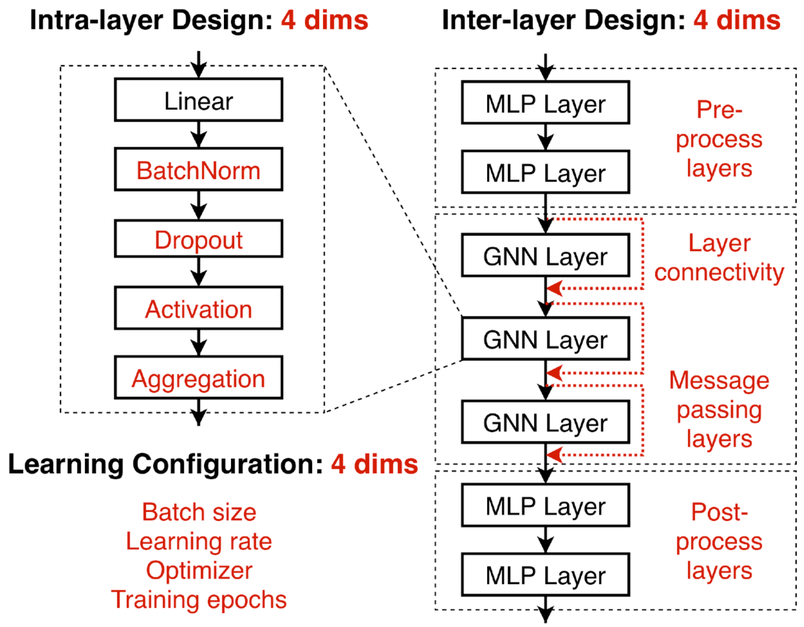
(Nearly) all real-world graphs are heterogeneous!

Heterogeneous Graphs

Overview

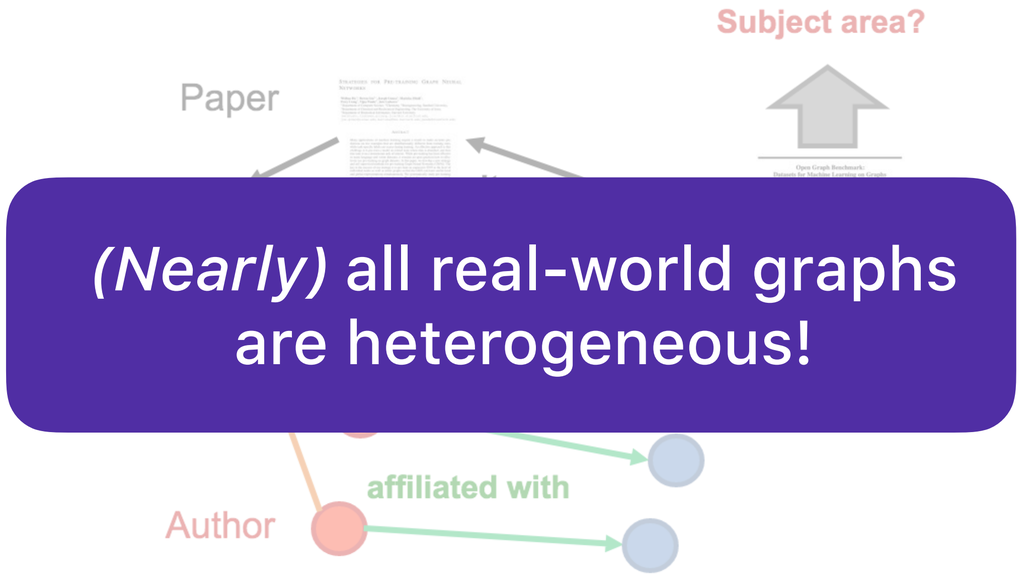


Heterogeneous Graphs

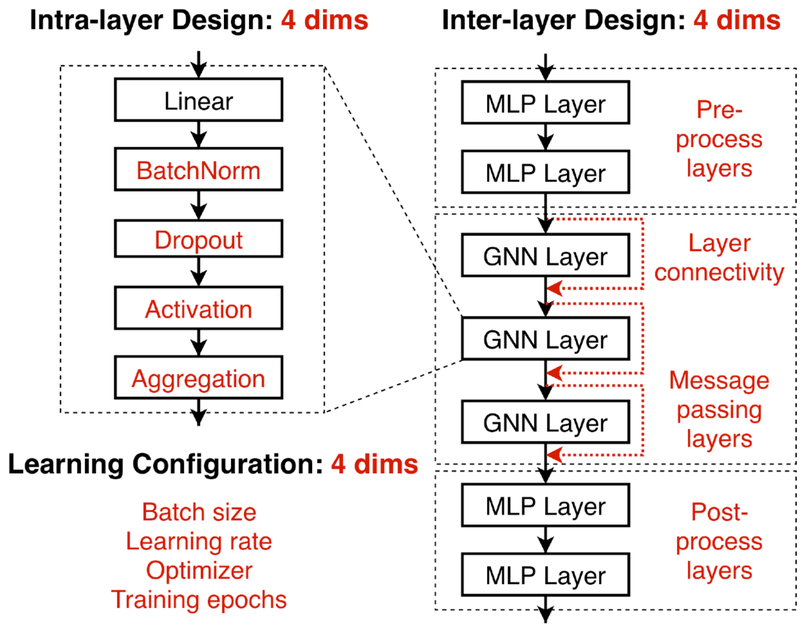


GraphGym

Overview



Heterogeneous Graphs



GraphGym

- ✓ Half-Precision Support
- ✓ *.`profile` for **benchmarking runtimes** and **memory consumptions** of GNNs
- ✓ A variety of new **operators, models, datasets** and **examples**

Heterogeneous Graph Support

Heterogeneous graph learning is notoriously challenging

Heterogeneous Graph Support

Heterogeneous graph learning is notoriously challenging

- **Different input feature distributions** across node and edge types
- **Necessity of learning node/edge type dependent representations**
  non-shared weights across different node and edge types
  bipartite message passing
- **Heterogeneous scalability approaches**
  Relational-wise neighborhood sampling
- **Complicated implementation**
  requires sequentially iterating over different node and edge types
  involves keeping track of different input feature dimensionalities

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PyG makes working with heterogeneous graphs a breeze

Heterogeneous Graph Support

Data Storage

Holds information about different node and edge types in **individual containers**

Edge types are described by a **triplet** of **source node**, **relation** and **destination node type**

Transformations enhance the graph for message passing, *e.g.*, by *adding reverse edges*

```python
from torch_geometric.data import HeteroData

data = HeteroData()

data['user'].x = ...  # User node feature matrix
data['product'].x = ...  # Product node feature matrix

# Connecting user and product nodes via "buys" relation:
data['user', 'buys', 'product'].edge_index = ...  # [2, num_edges]

# Adding reverse edges:
from torch_geometric.transforms import ToUndirected

data = ToUndirected()(data)
```

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We provide a **full example** for **loading raw `*.csv` files** in the **documentation**

Heterogeneous Graph Support

Heterogeneous Graph Neural Networks

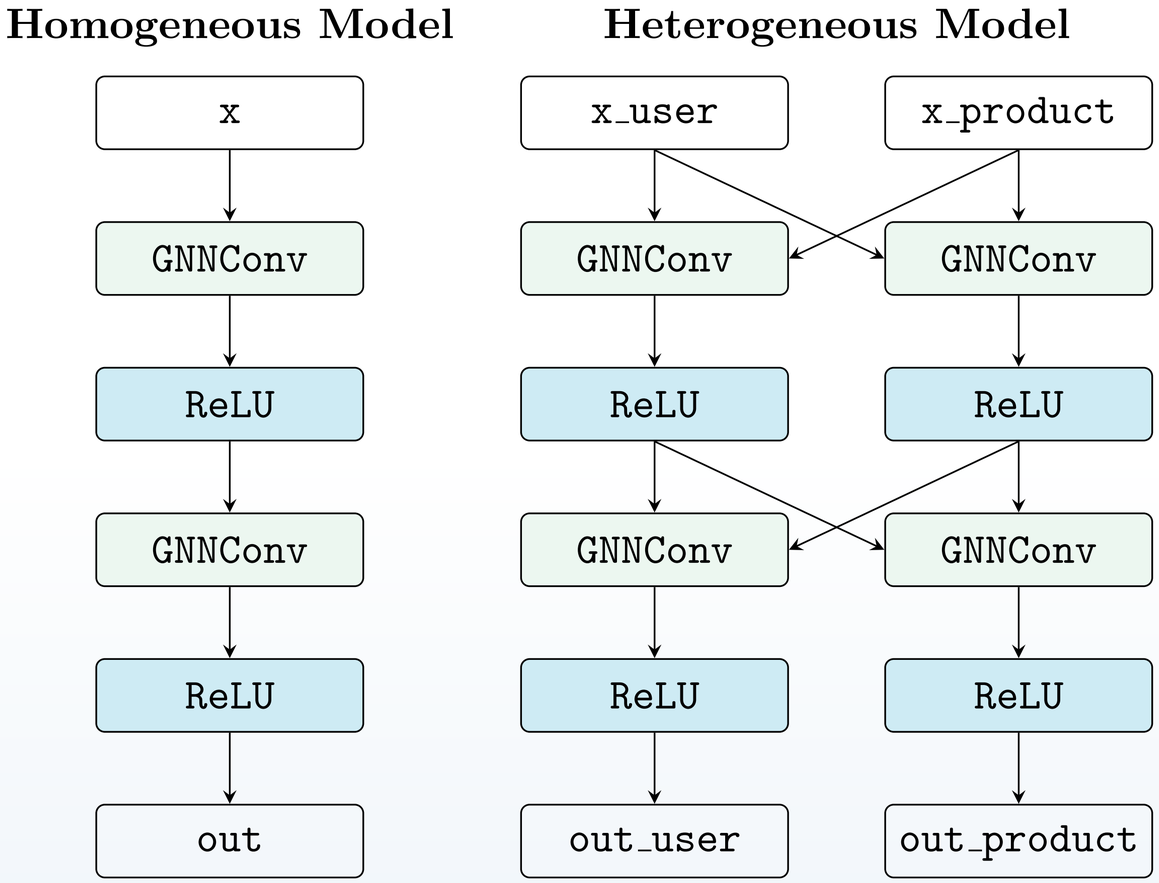
A **homogeneous GNN** can be converted to a **heterogeneous one** by learning **distinct parameters** for **each individual edge type:**

A custom GNN for each relation

$$\mathbf{h}_i^{(\ell+1)} = \sum_{r \in \mathcal{R}} \mathrm{GNN}_\theta^{(r)} \left(\mathbf{h}_i^{(\ell)}, \{ \mathbf{h}_j^{(\ell)} : j \in \mathcal{N}^{(r)}(i) \} \right)$$

The number of relations

Relational-wise neighborhood



Heterogeneous Graph Support

Heterogeneous Graph Neural Networks

Rapid growth in the number of parameters *w.r.t* number of relations may lead to overfitting on rare relations

Basis-decomposition for regularization

A custom GNN for each basis

$$\mathbf{h}_i^{(\ell+1)} = \sum_{r \in \mathcal{R}} \sum_{b=1}^{B} \mathrm{GNN}_\theta^{(b)} \left(\mathbf{h}_i^{(\ell)}, \{ a_{r,b}^{(\ell)} \cdot \mathbf{h}_j^{(\ell)} : j \in \mathcal{N}(i) \} \right)$$

The number of bases

Relational-depend trainable coefficients

Heterogeneous Graph Support

PyG can **automatically convert homogeneous GNNs to heterogeneous ones**

```
to_hetero(model (node_types, edge_types)):
to_hetero_with_bases(model (node_types, edge_types)):
```

1. **Duplicates** message passing modules for **each edge type**
2. **Transforms** the **underlying computation graph** so that messages are exchanged along **different edge types**
3. Uses **lazy initialization** (–1) to handle different **input feature dimensionalities**

```python
from torch_geometric.nn import GAT, to_hetero

model = GAT(in_channels=-1, hidden_channels=64,
            out_channels=72, num_layers=2)

model = to_hetero(model, (node_types, edge_types))

out = model(data.x_dict, data.edge_index_dict)
```

Heterogeneous Graph Support

Heterogeneous Graph Samplers

Scaling up heterogeneous GNNs
to large-scale graphs with ease
via **relational neighbor sampling**

Only requires a few lines
of code change!

```python
from torch_geometric.datasets import OGB_MAG
from torch_geometric.loader import NeighborLoader

data = OGB_MAG(path)[0]

loader = NeighborLoader(
    data,
    num_neighbors={key: [15, 10] for key in data.edge_types},
    batch_size=128,
    input_nodes='paper')

for batch in loader:
    model(batch.x_dict, batch.edge_index_dict)
```

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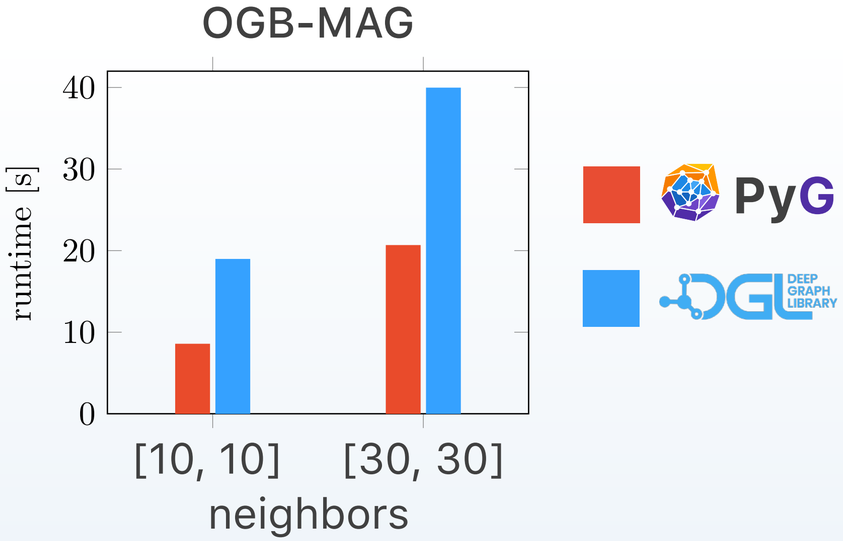


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Heterogeneous Graph Support

- A **tutorial** introducing **all newly released heterogeneous graph features**
- A **tutorial** showcasing how to **load heterogeneous graphs** from **raw `*.csv` files**
- **Heterogeneous graph transformations**
- **Conversion** from **heterogeneous graphs** to **homogeneous "typed" graphs**
- A **generic wrapper** (`HeteroConv`) for computing heterogeneous graph convolution via **different message passing operators**
- **Lazy initialization** (`-1`) for all message passing operators in **PyG**
- A variety of **heterogeneous GNN examples**, including an example for **scaling heterogeneous graph models** via **PyTorch Lightning**
- Dedicated **heterogeneous graph operators** (`HGTConv`) and **samplers** (`HGTLoader`)

`https://pytorch-geometric.readthedocs.io`
`/pyg-team/pytorch-geometric/releases`

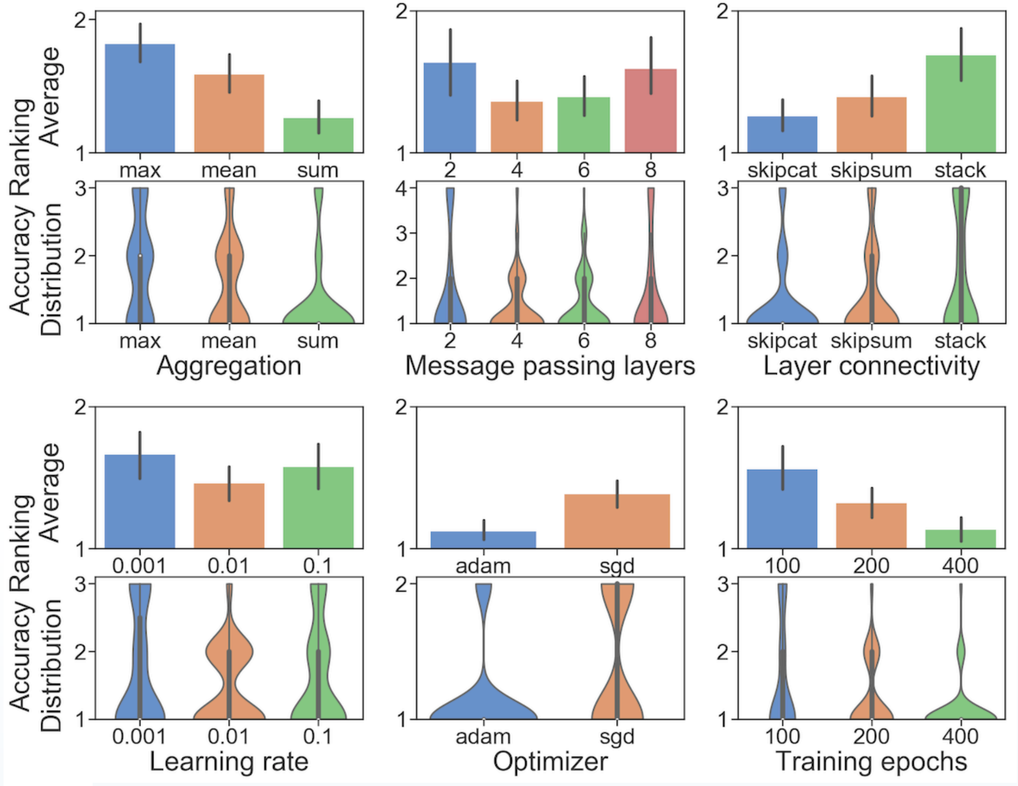
GraphGym

Design Space Exploration with GraphGym

Which GNN is the best for your given task?

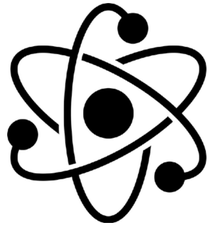
GraphGym aims to design and train GNNs from **configurations**, using a **modularized pipeline:**

- **Standardized** GNN implementation/evaluation
- **Design space exploration** via simple interfaces to try out thousands of GNN architectures **in parallel**
- Hyper-parameter search and visualizations



Future Plans

Future Plans



Temporal Graphs

- *(Nearly)* all real-world graphs are **inherently dynamic**
- Support for **addition** and **removal** of **nodes** and **edges**
- Integration of **temporal Graph Neural Networks**
- **Real-Time In-Stream Inference**

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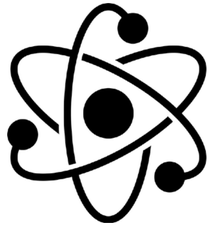

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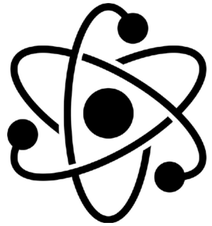
Distributed Data

- While distributed training is possible, **distributing data is currently a user task**
- Scaling to **billions of nodes** via distributing input data
- **Partitioning** input node and edge features

Future Plans



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Auto-Scaling

- **PyG** should **automatically determine the best scalability approach** for the given task
- Write GNNs in **full-batch mode** and let **PyG** figure out the rest
- **GNNAutoScale** (ICML 2021)

Conclusion

PyG bundles the **state-of-the-art** in **Graph Representation Learning**

- ✓ 50+ **GNN architectures**
- ✓ 200+ **benchmark datasets**
- ✓ Dedicated **sparsity-aware CUDA kernels**
- ✓ **Multi-GPU** support
- ✓ **Half-Precision** support
- ✓ Support for **scalability techniques**
- ✓ **Heterogeneous graph** support
- ✓ GNN Design Space Exploration

We are constantly encouraged to make PyG even better!

dortmund university

Stanford University

team@pyg.org

https://pyg.org

/pyg-team/pytorch-geometric


```
conda install pyg -c pyg
```