PyG

Progress and Future

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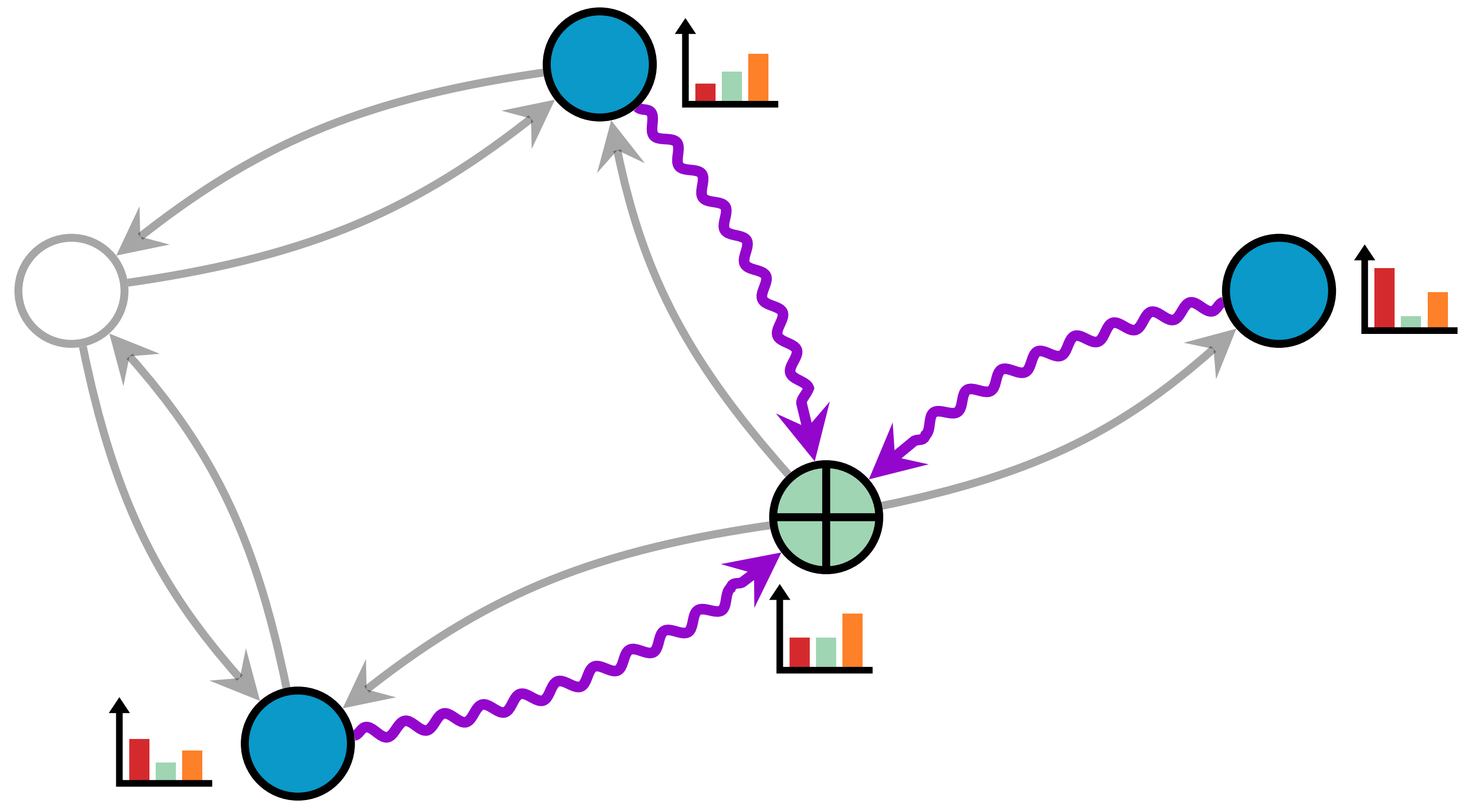
https://pyg.org

/pyg-team/pytorch-geometric


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

Graph Neural Networks



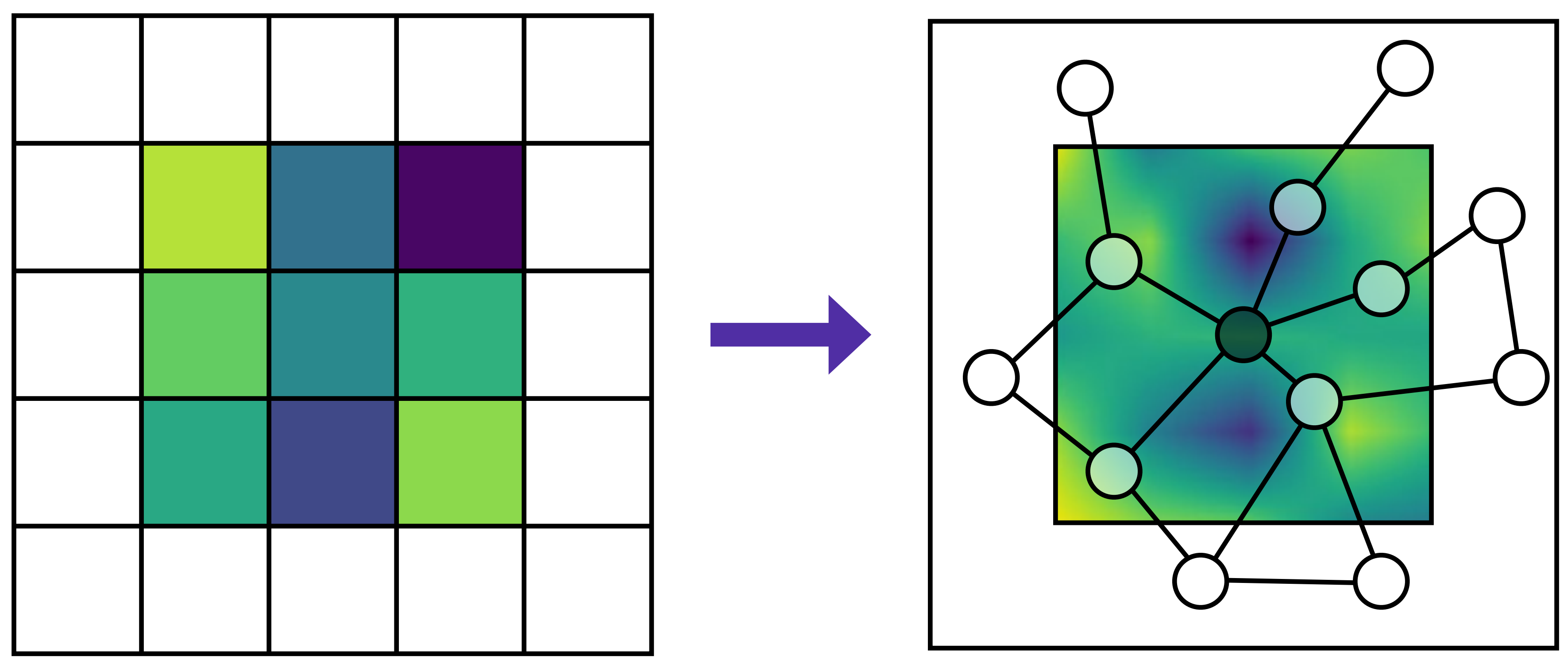
Message Passing Scheme

- ✓ **Generalization** of *any* **neural network architecture**
- ✓ **Data-dependent** computation

A **new paradigm** of *how* we define **neural networks!**

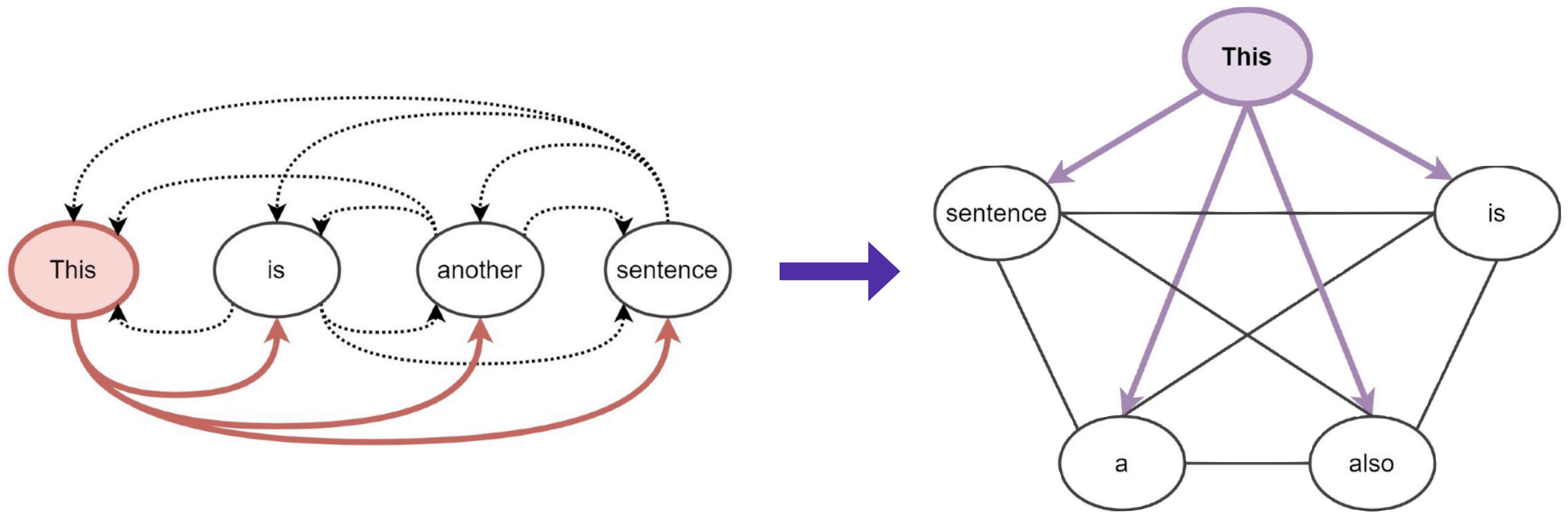
From **CNNs** *to* **GNNs**

Message Passing via **continuous kernels**



From **Transformers** *to* **GNNs**

Message Passing within a **fully-connected graph**



Implementing **Graph Neural Networks** is **challenging**

- **Sparsity** *and* **irregularity** of the underlying data
  How can we effectively parallelize irregular data of potentially varying size?
- **Heterogeneity** of the underlying data
  numerical, categorical, image and text features, potentially over *different* types of data
- *Inherently* **dynamic**
  it is hard to find scenarios in which graphs will *not* change over time
- Various *different* **requests** on **scalability**
  sparse *vs.* dense graphs, many small *vs.* single giant graphs, ...
- Applicability to a set of *diverse* **tasks**
  node-level *vs.* link-level *vs.* graph-level, clustering, pre-training, self-supervision, ...

PyTorch Geometric

PyG *(PyTorch Geometric)* is the **PyTorch** library to **unify deep learning** on **graph-structured data**

- ✓ simplifies implementing and working with **Graph Neural Networks**
- ✓ bundles *state-of-the-art* **GNN architectures** and **training procedures**
- ✓ achieves *high* **GPU throughput** on sparse data of varying size
- ✓ suited for *both* **academia** and **industry**
  flexible, comprehensive, easy-to-use

Design Principles

Graph-based Neural Network Building Blocks

- ✓ Message Passing layers
- ✓ Normalization layers
- ✓ Pooling & Readout layers
- ✓ ...

In-Memory Graph Storage, Datasets & Loaders

- ✓ Support for heterogeneous graphs
- ✓ *200+* benchmark datasets
- ✓ *10+* sampling techniques

Graph Transformations & Augmentations

- ✓ Graph iffusion
- ✓ Missing feature value imputation
- ✓ Mesh and Point Cloud support

Examples & Tutorials

- ✓ Learn practically about GNNs
- ✓ Videos, Colabs & Blogs
- ✓ Application-driven Graph ML Tutorials

Design Principles

```
dataset = Reddit(root_dir, transform)

loader = NeighborLoader(dataset, num_neighbors=[25, 10])

class GNN(torch.nn.Module):
    def __init__(self):
        self.conv1 = SAGEConv(F_in, F_hidden)
        self.conv2 = SAGEConv(F_hidden, F_out)

    def forward(x, edge_index):
        x = self.conv1(x, edge_index)
        x = x.relu()
        x = self.conv2(x, edge_index)
        return x

for data in loader:
    data = data.to(device)
    out = model(data.x, data.edge_index)
    loss = criterion(out, data.y)
    loss.backward()
    optimizer.step()
```

PyG is *highly* modular

- ✓ Access to *200+* **datasets** and *50+* **transforms**
- ✓ Access to a *variety* of **mini-batch loaders**
  Node-wise sampling, Subgraph-wise sampling, graph-wise batching
- ✓ Access to *80+* **GNN layers, normalizations** and **readouts** as neural network building blocks
  SAGEConv, GCNConv, GATConv, GINConv, PNAConv, ...

  and

  20+ **pre-defined models**
  GraphSAGE, GCN, GAT, GIN, PNA, SchNet, DimeNet, ...
- ✓ Access to regular PyTorch **loss functions** and **training routines**
  Classification, Regression, Self-Supervision, ...
  Node-level, Link-level, Graph-level

Design Principles

PyG is PyTorch-on-the-rocks

- ✓ **PyG** is framework-specific
  - allows us to make use of *recently released* features right away
  - `TorchScript` for **deployment**, `torch.fx` for **model transformations**
- ✓ **PyG** keeps **design principles** *close* to vanilla PyTorch
  - If you are familiar with PyTorch, you already know most of **PyG**
- ✓ **PyG** fits nicely into the **PyTorch ecosystem**
  - **Scaling up** models via **PyTorch Lightning**
  - **Explaining** models via **Captum**

Ecosystem

The PyG ecosystem

PyTorch Geometric Temporal

DiveIntoGraphs

PyTorch Geometric Signed Directed

Quiver

PyGOD

Graphein

... and *many* more!

PyG

Progress and Future

Timeline

FAST GRAPH REPRESENTATION LEARNING WITH PYTORCH GEOMETRIC

- ✓ Stanford Partnership
- ✓ Heterogeneous GNNs

- ✓ *Principled* **Aggregations**
- ✓ **Scalable Link Prediction**
- ✓ **Temporal** Samplers
- ✓ …

- ✓ Accelerations
- ✓ Scalability
- ✓ …

Paper Release
March'19

PyG 2.0 Release
Sep'21

PyG 2.1 Release
Aug'22

PyG 2.2 Release
Nov'22

Open-Sourced
Nov'17

OGB Collaboration
Feb'20

Partnership Acquisition
'21

- ✓ **Kumo.AI** Partnership
- ✓ **NVIDIA** Partnership
- ✓ **Intel** Partnership

Announcements

Major Architecture Change

A *new* **GNN engine:** `pyg-lib`

Joint effort across *many* different partners

New Optimizations

Improved **GNN design**
via
principled aggregations

Improved **scalability**
and
pluggable graph backend support

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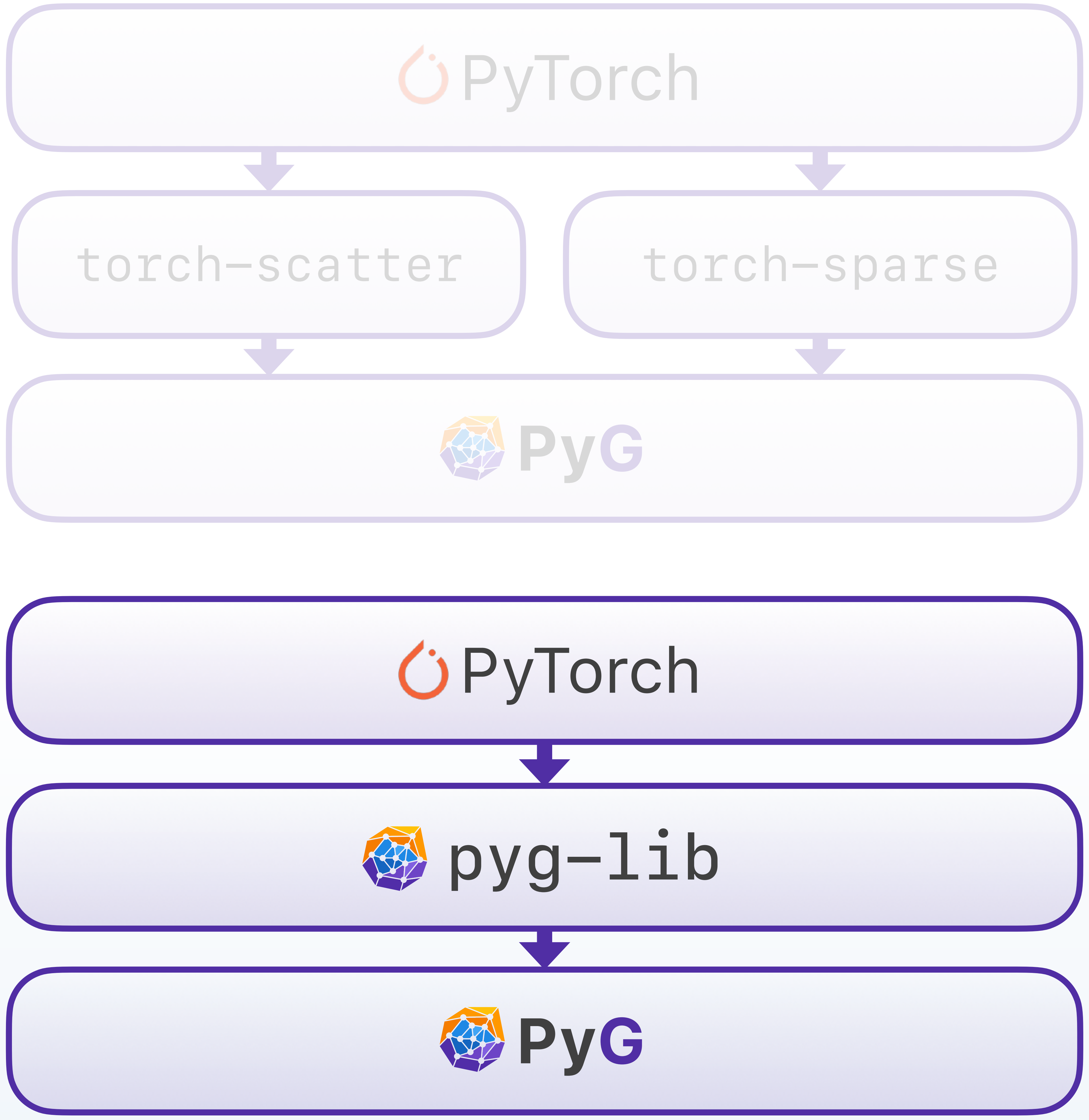
Accelerating PyTorch Geometric



`pyg-lib`: A unified GNN engine for **optimized low-level graph routines**

`/pyg-team/pyg-lib`

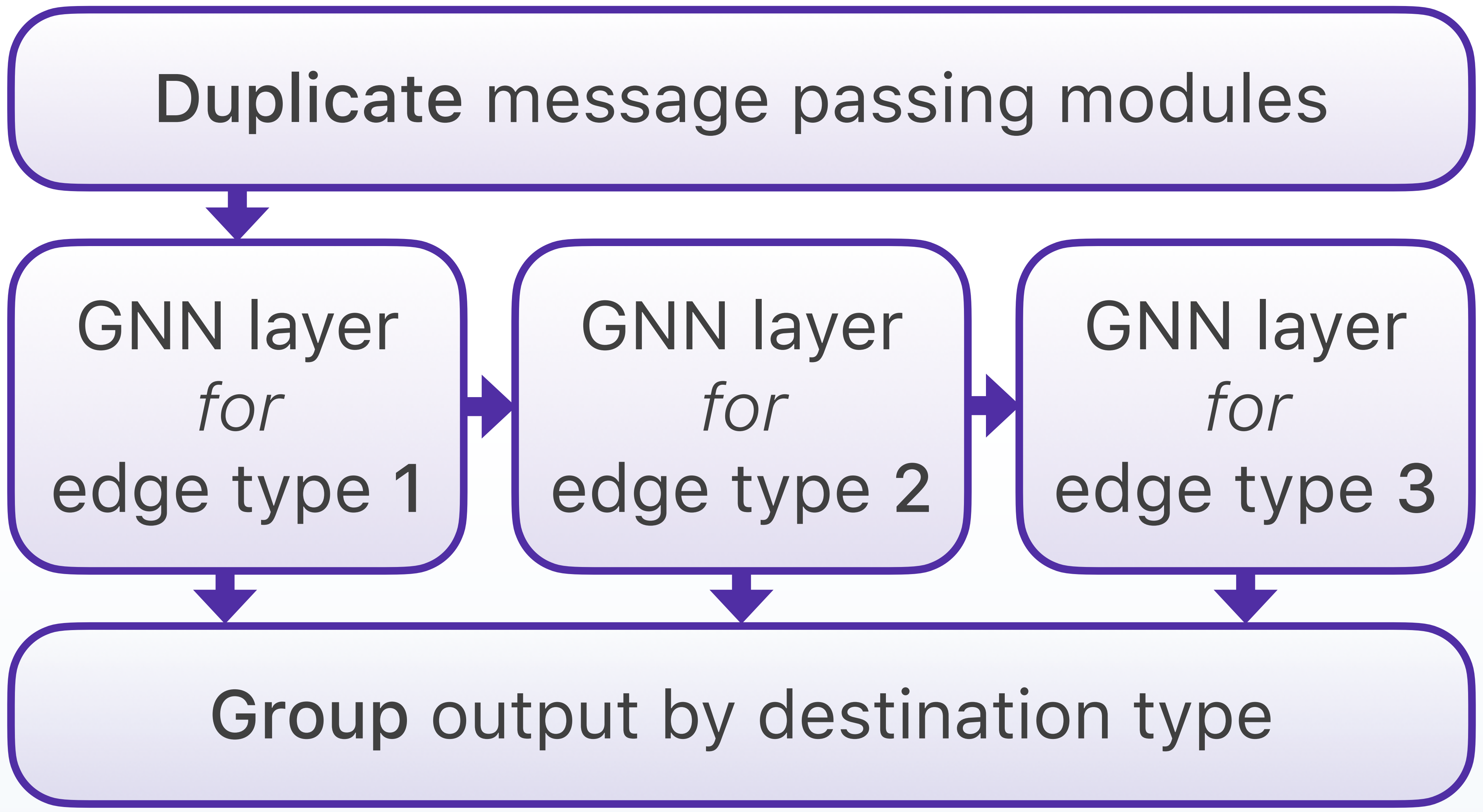
- ✓ **Joint effort of** Kumo, NVIDIA, Intel & PyTorch
- ✓ *Accelerating* **graph sampling routines**
- ✓ *Accelerating* **heterogeneous GNNs**
- ✓ *Accelerating* **sparse aggregations**
- ✓ **Speed-ups** with *no* line of code change

Accelerating Heterogeneous GNNs

PyG `2.0` integrated **heterogeneous graph** *and* **GNN** support

- `HeteroData`: in-memory storage
- **Metapath** transformations
- **Heterogeneous graph samplers**
- **Heterogeneous GNN layers**
- **Lazy initialization** to *elegantly* support feature dimensions of *varying* size
- `to_hetero()`: A *principled* way to bring *recent* **advancements of GNNs** to **heterogeneous graphs** *right away*

`to_hetero(model)`

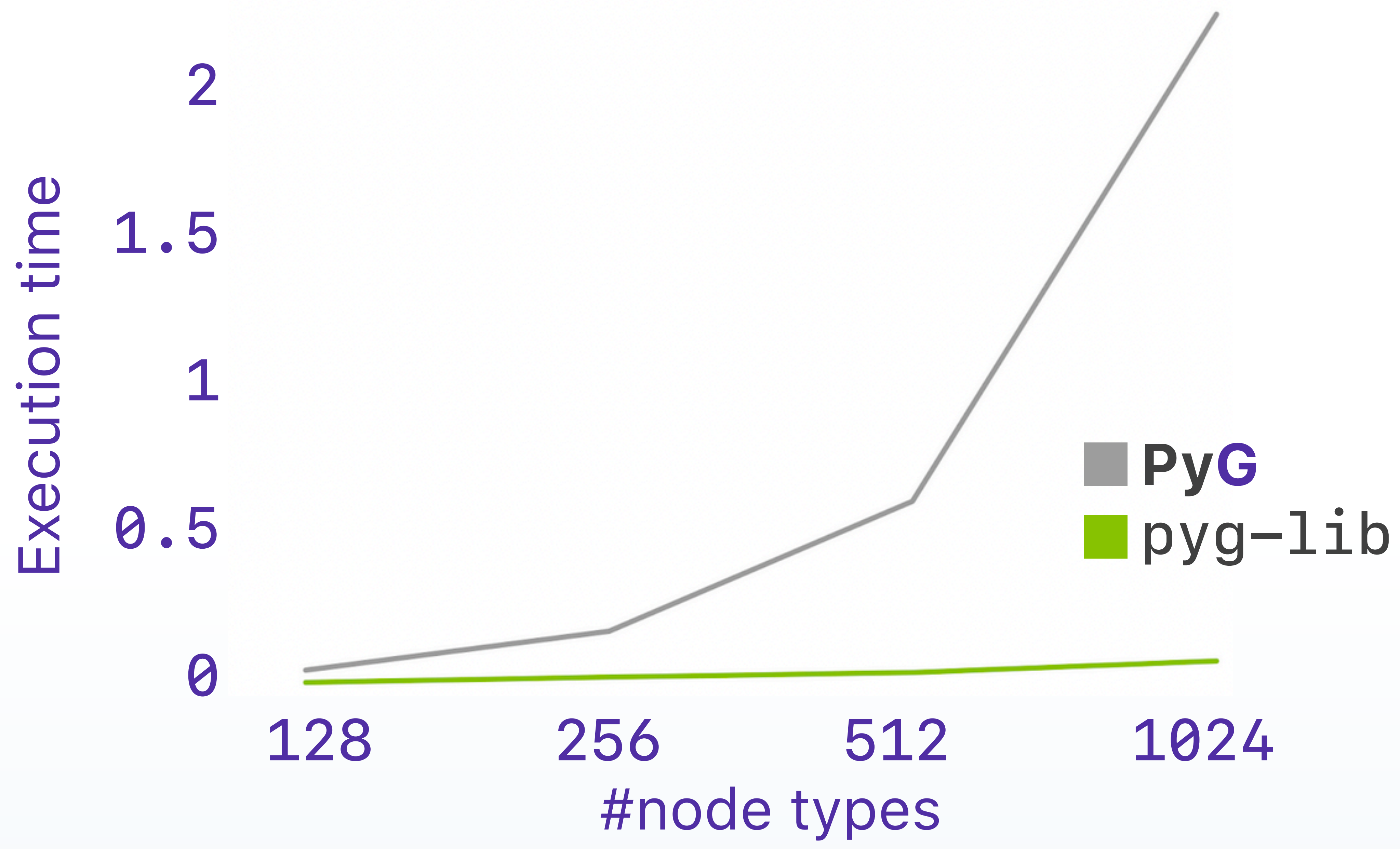


Accelerating Heterogeneous GNNs

`to_hetero()` is a **powerful** tool but lacks **parallelism** *across* **edge types**

`pyg-lib` supports *concurrent* **type-dependent transformations** via **NVIDIA CUTLASS** integration

- ✓ **Flexible** to implement *most* heterogeneous GNN operators with
- ✓ **Efficient**, even on *sparse* types or on a *large number* of types

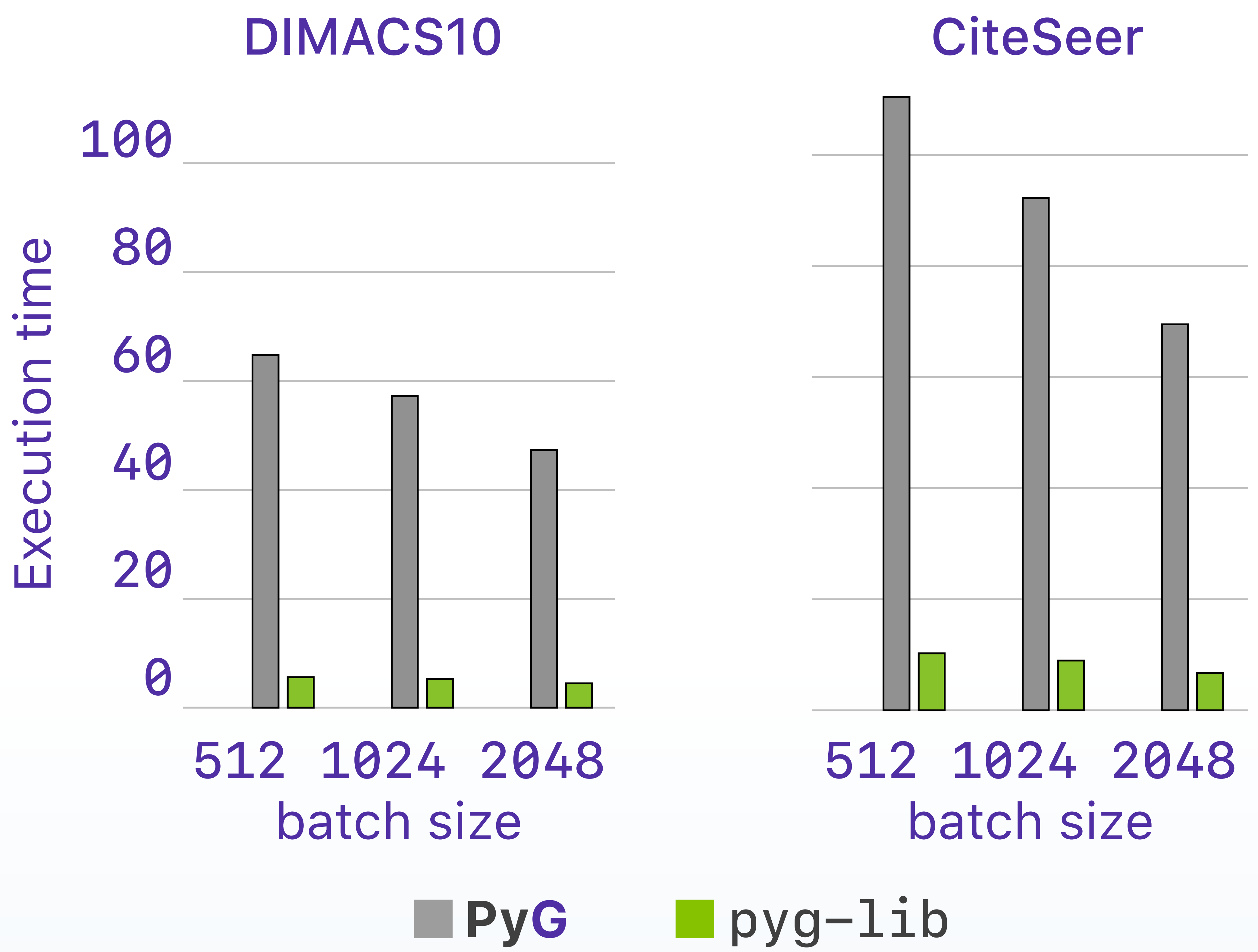


Find out *more* in the **Accelerating PyG with NVIDIA GPUs** talk *later*!

Accelerating Graph Samplers

`pyg-lib` leverages a *variety* of techniques to further accelerate **neighbor sampling routines**

- ✓ **Pre-allocation** of **random numbers**
- ✓ **Vector-based mapping** of nodes for *smaller* node types
- ✓ *Faster* **hashmap** implementation
- ✓ *10x* to *15x* **speed-ups**



Find out *more* in the **Accelerating PyG with Intel CPUs talk** *later*!

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Improved **GNN design**
via
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Improved **scalability**
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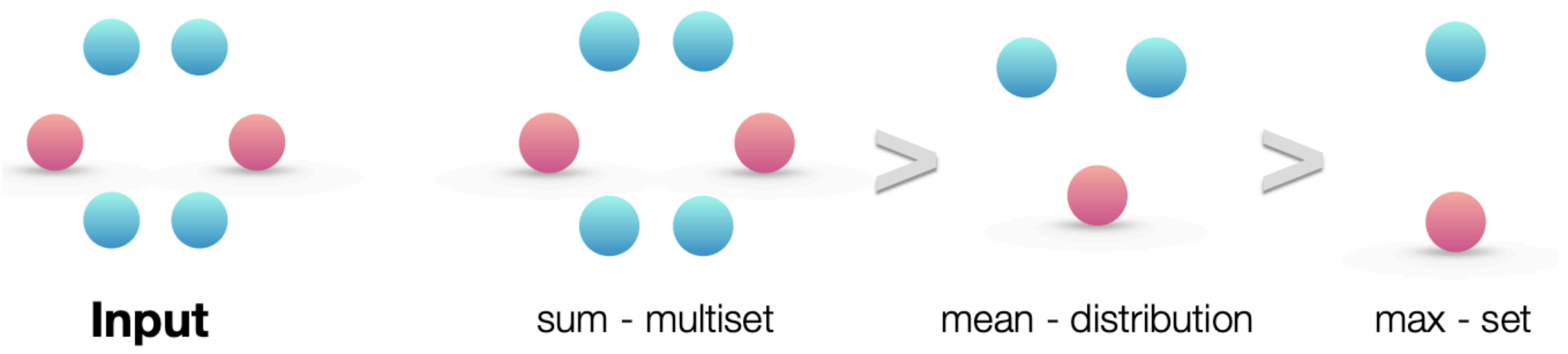
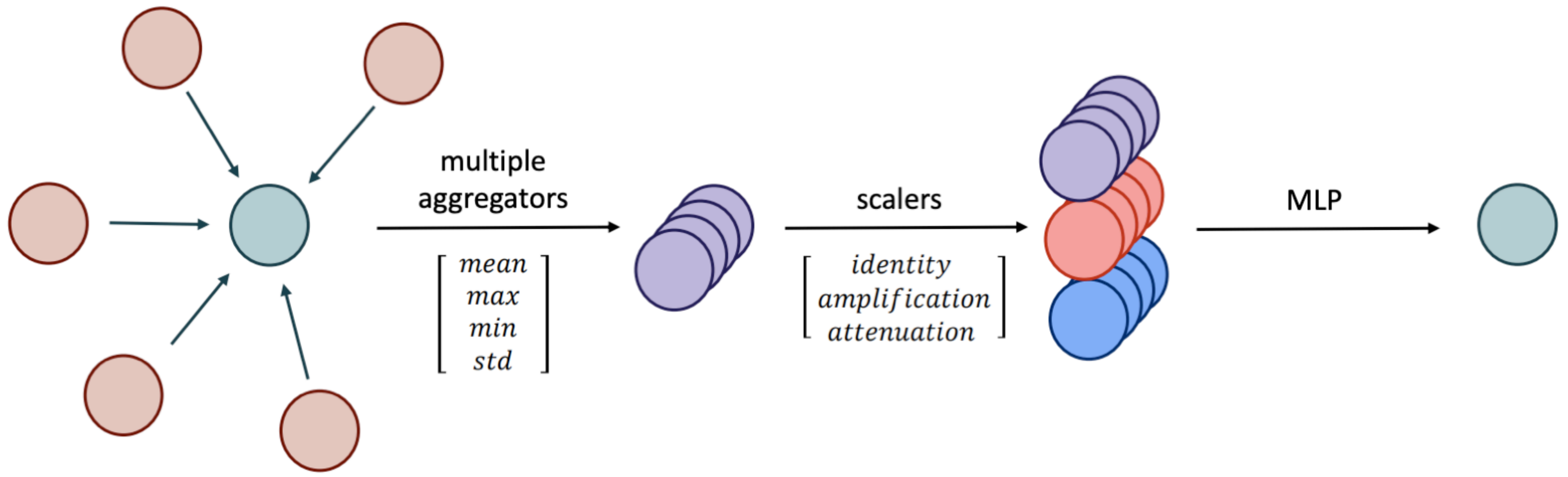
Principled Aggregations

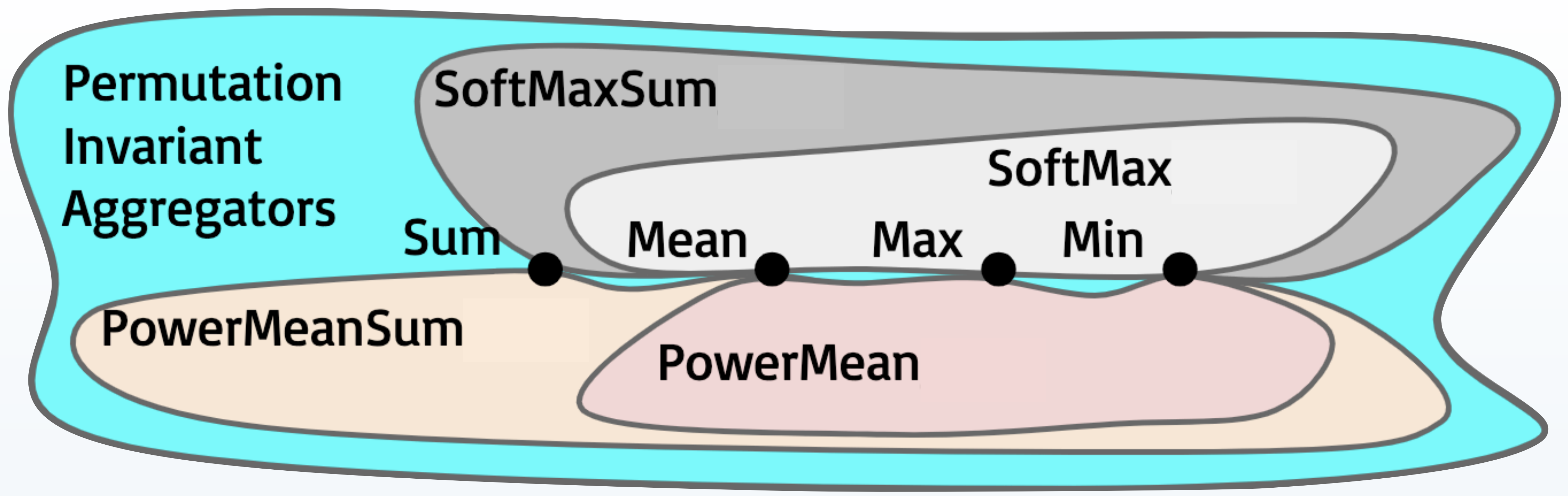
Choice of **neighborhood aggregation** is a *central* topic in **Graph ML research**



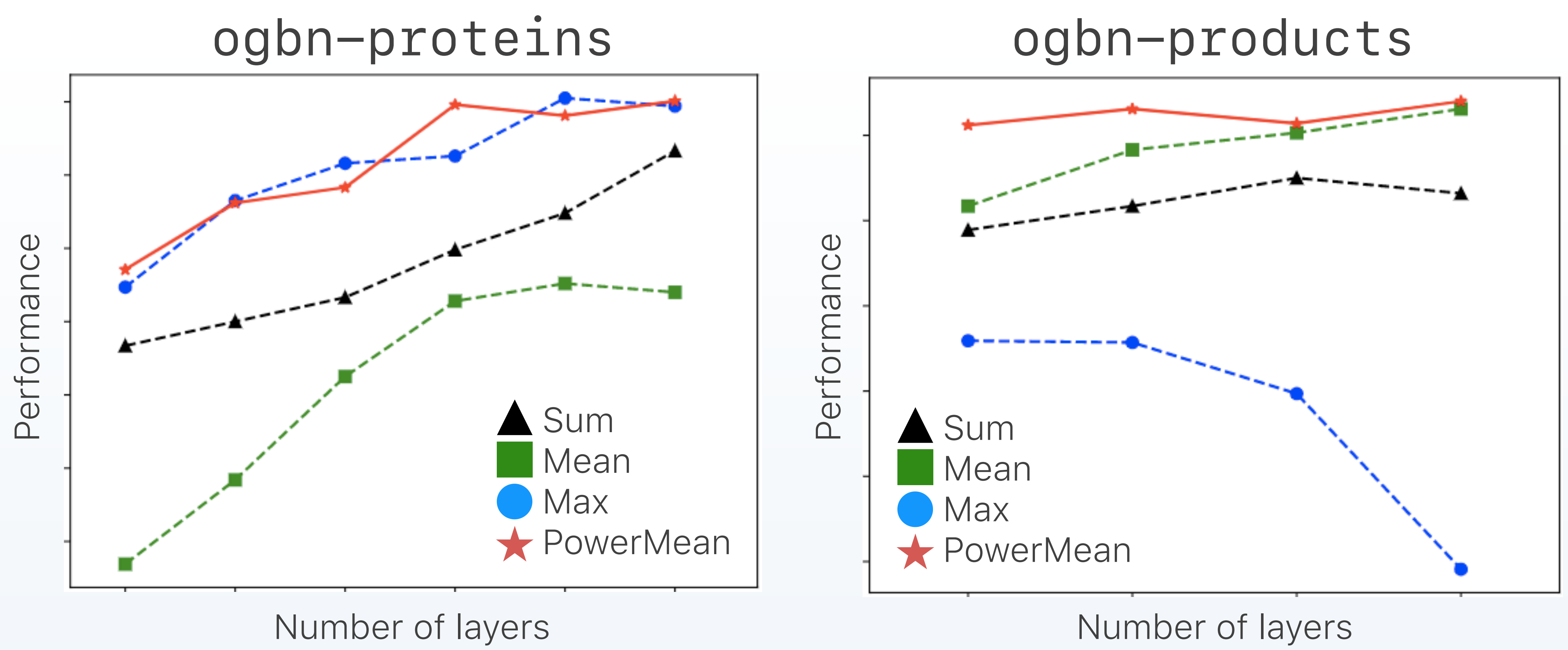
Xu *et al.*: How Powerful Are Graph Neural Networks?



Corso *et al.*: Principal Neighborhood Aggregation for Graph Nets



Li *et al.*: Deeper-GCN: All You Need to Train Deeper GCNs



Principled Aggregations

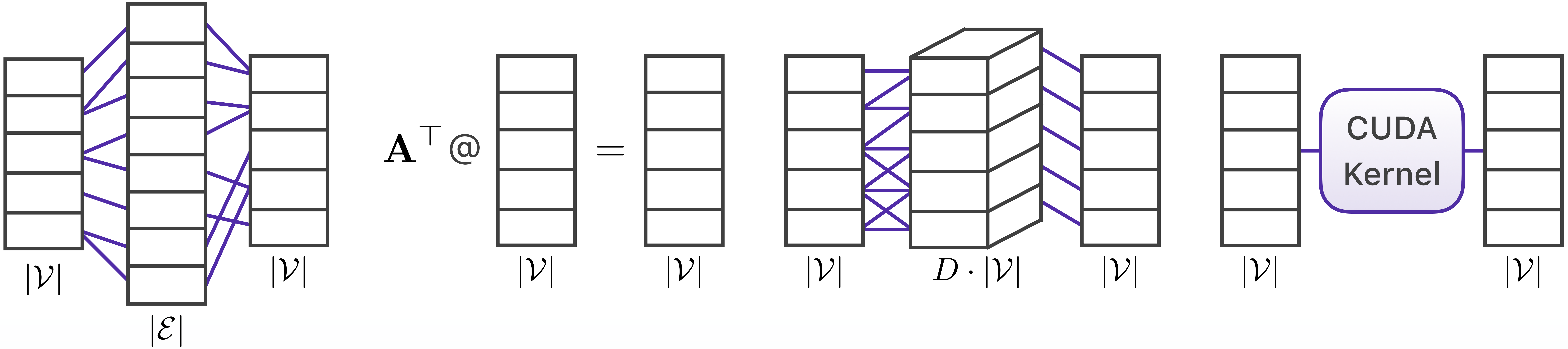
```
# Simple aggregations:
mean_aggr = aggr.MeanAggregation()
max_aggr = aggr.MaxAggregation()

# Advanced aggregations:
median_aggr = aggr.MedianAggregation()

# Learnable aggregations:
softmax_aggr = aggr.SoftmaxAggregation(learn=True)
powermean_aggr = aggr.PowerMeanAggregation(learn=True)

# Exotic aggregations:
lstm_aggr = aggr.LSTMAggregation()
sort_aggr = aggr.SortAggregation(k=4)

# Use within message passing:
conv = MyConv(aggr=[median_agr, lstm_aggr])

# Use for global pooling:
h_graph = sort_aggr(h_node, batch)
```

PyG makes the concept of aggregations a *first-class* **principle**

- ✓ Access to *all* kinds of **simple**, **advanced**, **learnable** and **exotic aggregations**
  Median, Softmax, Attention, LSTM, ...
- ✓ **Fully-customize** and **combine aggregations** within `MessagePassing` *or* for **global pooling**
- ✓ Aggregations will pick up the *best* **format** to **accelerate computation**
  scatter reductions, degree bucketing, ...
- ✓ Further **optimization** *via* **fusion** possible *(TBD)*

Principled Aggregations

The *different* **flavors** of **implementing aggregations**



Gather & Scatter

- very flexible 🤗
- fast for sparse graphs 🤗
- memory-inefficient 😭

PyG >= 0.1

Sparse MatMul

- less flexible 😭
- very fast 🤗
- memory-efficient 🤗

PyG >= 1.6

Degree Bucketing

- any aggregation 🤗
- memory-inefficient 😭
- padding/seq. iteration 😭

PyG >= 2.1

Individual Kernel

- not flexible at all 😭
- memory-efficient 🤗
- very fast 🤗

PyG >= 2.2

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Scalable Link Prediction

PyG simplifies implementing *scalable* **link prediction tasks**

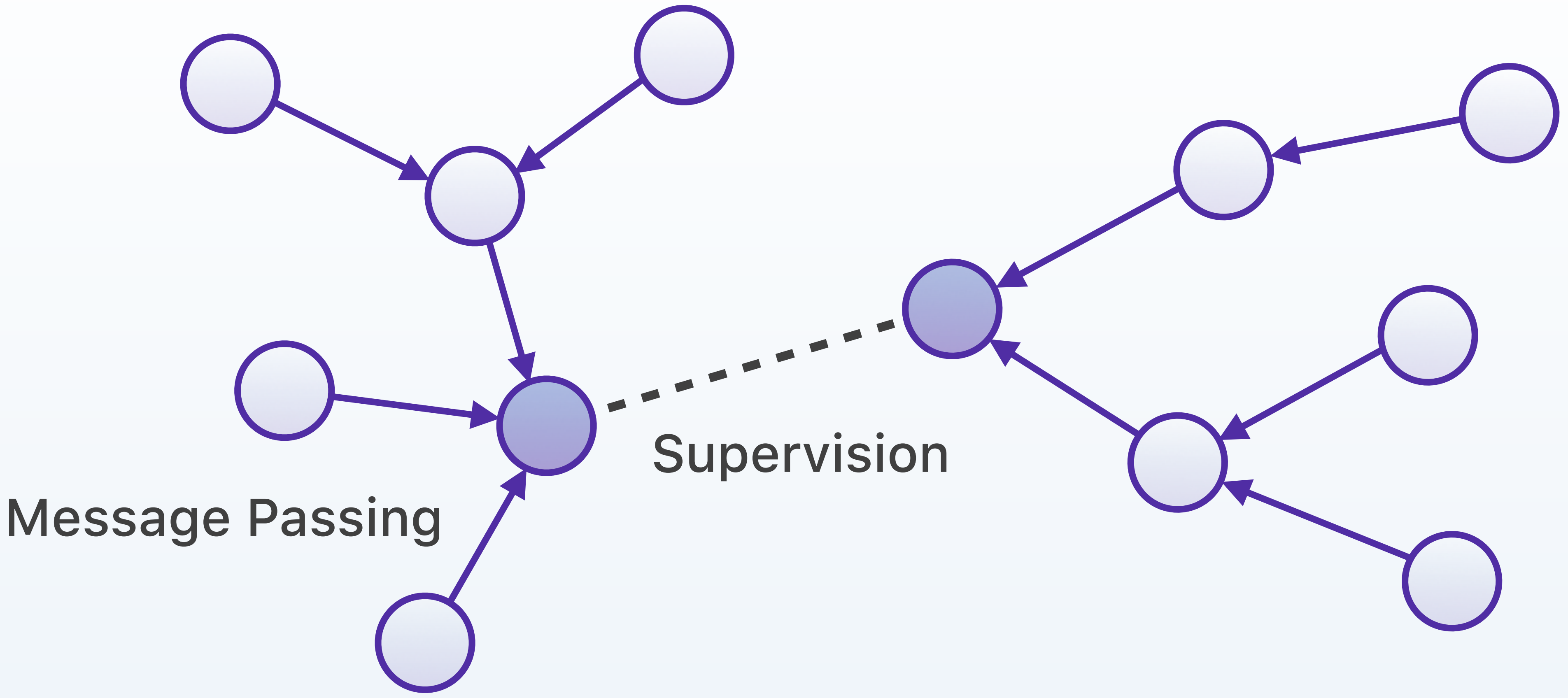
```
data = Reddit(root_dir)

train_data, _, _ = RandomLinkSplit(data)

train_loader = LinkNeighborLoader(
    train_data, num_neighbors=[25, 10])

for train_data in train_loader:
    ...
    h = model.encode(train_data.x, train_data.edge_index)
    pred = model.decode(h, train_data.edge_label_index)
    loss = criterion(pred, train_data.edge_label)
    ...
```

- ✓ **Separation** between **message passing edges** `edge_index` and **supervision edges** `edge_label_index`
- ✓ Only *minor* changes required to **auto-scale your link prediction model**
- ✓ **Sampler** creates a **unified subgraph** by **sampling** from *both* **endpoints**



Out-of-Memory and Distributed Backend Support

Previously, **PyG** was limited to *single-node in-memory* datasets

```python
class MyFeatureStore(FeatureStore):
    def get_tensor(self, attr):
        pass  # Implement feature access


class MyGraphStore(GraphStore):
    def sample_from_nodes(self, index):
        pass  # Implement node-wise sampling

    def sample_from_edges(self, index):
        pass  # Implement edge-wise sampling
```

With PyG, we aim **to support** *any* **backend** by providing `FeatureStore` *and* `GraphStore` **abstractions**

- ✓ Disentangles **feature fetching** *from* **graph sampling routines**
- ✓ Allows *for* **distributed server/client architectures**
- ✓ Allows *for* **out-of-memory backends**, *e.g.*, via **memory-mapped I/O** *or* by connecting to **graph databases**

Find out *more* in the **Scaling-up PyG** talk *later*!

Additional Highlights

Automatic Mixed Precision

```
with torch.*.amp.autocast():
    out = model(data.x, data.edge_index)
```

Temporal Graph Samplers

```
loader = NeighborLoader(
    data, num_neighbors=[25, 10], time= ... )
```

Explainability

Captum

Explain predictions across *any* **GNN model, dataset,** and **task** *out-of-the-box*

Model Milestones

- **Deep GNNs** with *1000+* layers
  Li *et al.*: Training Graph Neural Networks with 1000 Layers
- GNNs on **heterophily graphs**
  Lim *et al.*: Large Scale Learning on Non-Homophilous Graphs: New Benchmarks and Strong Simple Methods
- ... and *many* more!

Conclusion

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

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

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

We are constantly encouraged to make PyG *even* better!