Graph Neural Networks II

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Message Passing

Input:

- Graph $G = (V, E)$
- Node Features $X_V : V \to \mathbb{R}^d$
- Edge Features $X_E : E \to \mathbb{R}^{d'}$ (optional)

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- Update latent vertex embedding $h^\ell(v) \in \mathbb{R}^{d^\ell}$ in each layer ℓ.
- The update depends on the states of the neighbors.
- Use shared local neural network for the update.

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Elements of a GNN Layer [Wu et al., 2020]:

- Trainable functions $\mathbf{M}^\ell$, $\mathbf{U}^\ell$
- Aggregation function $\bigoplus$ (Sum, Mean, Max,. . .)

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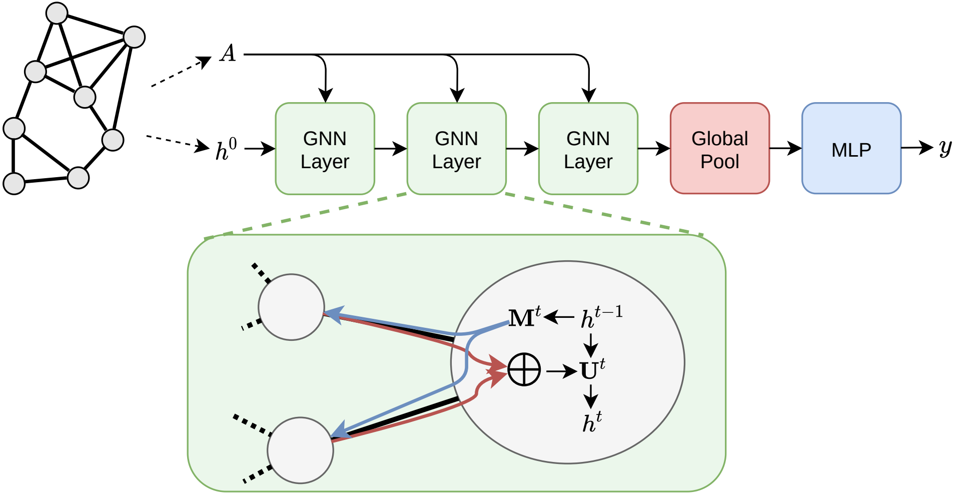
Function computed by the layer:

$$h^\ell(v) = \mathbf{U}^\ell \left(h^{\ell-1}(v), \bigoplus_{u \in \mathcal{N}(v)} \mathbf{M}^\ell \left(h^{\ell-1}(u), X_E(vu) \right) \right)$$

Graph Neural Networks



Implementing Message Passing

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Better Solution: **Scatter Operations**

PyTorch Scatter

Open Source Torch Extension[1].

Compatible with CUDA and Backpropagation.

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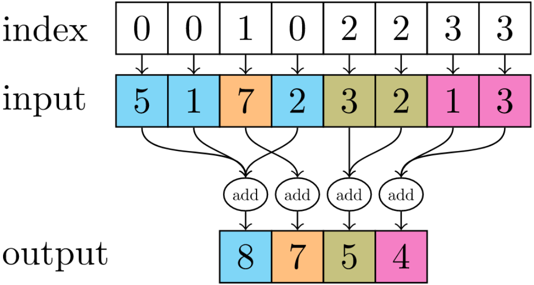
Enables aggregation of input with index list:



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PyTorch Scatter Example

$$x = \begin{pmatrix} 0 & 2 \\ 1 & 0 \\ 1 & 1 \\ 3 & 5 \\ 0 & 1 \end{pmatrix}$$

$$\mathrm{idx} = [0, 1, 0, 2, 2]$$

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4. Graph label $y \in \mathbb{R}^c$

my guess
j'th column gives you source
and target of j'th edge
(u)
(v)

Message Passing with Scatter

Given: $H^{(\ell-1)} \in \mathbb{R}^{|V| \times d_h}, \quad X_E \in \mathbb{R}^{2|E| \times d'}, \quad \text{idx}_E \in \{0, \dots, |V|-1\}^{2 \times 2|E|}$

Compute:

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$$H^{(\ell)} = \mathbf{U}\left(H^{(\ell-1)}, Z^{(\ell)}\right)$$

Batching Sparse Graphs

Given: Batch of training graphs $(\text{idx}_{E_1}, X_{V_1}, X_{E_1}, y_1), \ldots, (\text{idx}_{E_b}, X_{V_b}, X_{E_b}, y_b)$

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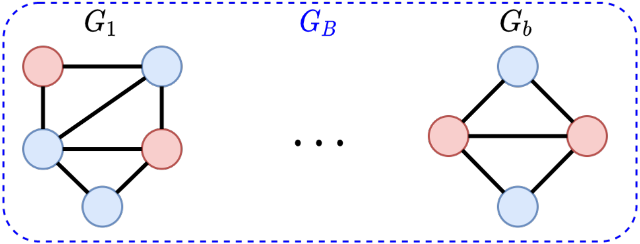

How do we combine these into one input for parallel processing?

Compute disjoint union $G_B = (V_B, E_B)$: $V_B = \bigcup_{i=1}^{b} V_i$, $E_B = \bigcup_{i=1}^{b} E_i$

Batching Sparse Graphs

Representation of the batched graph G_B:

1. $\mathrm{idx}_E \in \{0, \ldots, |V_B| - 1\}^{2 \times 2|E_B|}$
2. $X_{V_B} \in \mathbb{R}^{|V_B| \times d}$
3. $X_{E_B} \in \mathbb{R}^{|E_B| \times d'}$
4. $y_B \in \mathbb{R}^{B \times c}$
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Batching Sparse Graphs in PyTorch

Write custom collation function in Python:

- Input: $[(\mathrm{idx}_{E_1}, X_{V_1}, X_{E_1}, y_1), \ldots, (\mathrm{idx}_{E_b}, X_{V_b}, X_{E_b}, y_b)]$
- Output: $(\mathrm{idx}_{E_B}, X_{V_B}, X_{E_B}, y_B, \mathrm{batch\_idx})$
- Pass function to `DataLoader` as `collate_fn` parameter.

GNNs in Practice

Typical Hyperparameters:

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Most GNNs are relatively shallow and small (compared to CNNs, Transformers, etc.)

GNN Components

Update function **U**:

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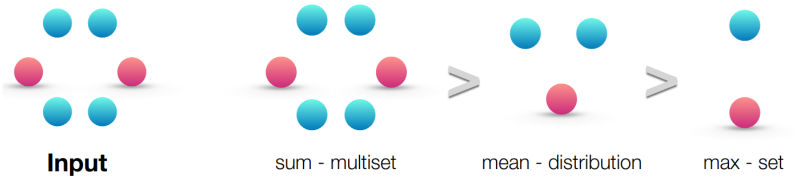
- Usually MLP with one or two layers
- If **U** has two layer, the second layer is usually linear

Message function **M**:

- If no edge features are given, simply use identity (like the GCN)
- If edge features are given, **M** should be non-linear.

Aggregation

Expressiveness of aggregation functions [Xu et al., 2019]:



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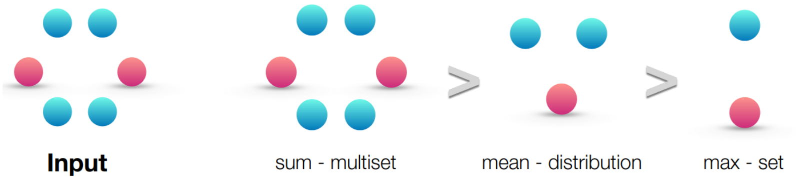

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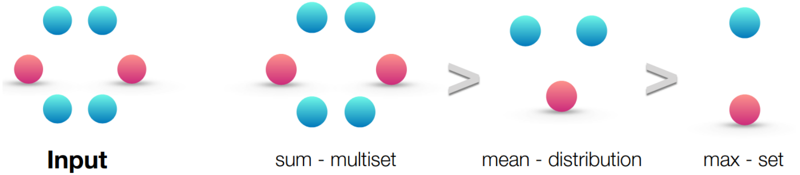

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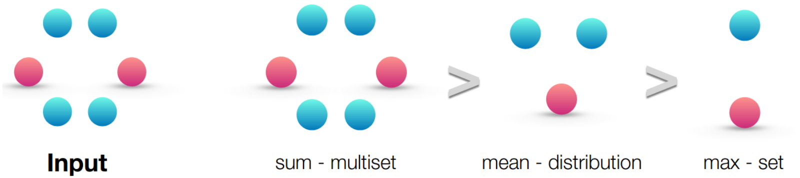

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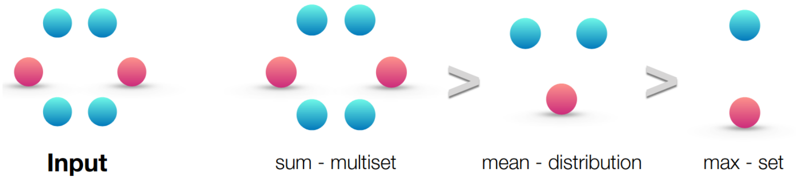

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More advanced: Predict edge weights with attention. [Veličković et al., 2018]

Special GNNs

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Heterogeneous GNNs:

- Heterogeneous graphs contain nodes of different types.
- Train different functions **U**, **M** for each type of node.

Standard Tricks

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Most of the standard tricks from Deep Learning also work for GNNs:

- Batch/Layer Normalization
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- Use Residual Connections:

$$h^{\ell}(v) = h^{\ell-1}(v) + \mathbf{U}^{\ell}\left(h^{\ell-1}(v), \bigoplus_{u \in \mathcal{N}(v)} \mathbf{M}^{\ell}\left(h^{\ell-1}(u), X_E(vu)\right)\right)$$

Virtual Nodes

Perform global pooling after each GNN layer and pass result back to nodes:

$$h^{\ell}(G) = \mathbf{V}^{\ell}\Big(\sum_{v \in V} h^{\ell}(v)\Big)$$
$$\tilde{h}^{\ell}(v) = h^{\ell}(v) + h^{\ell}(G)$$

Here, $\mathbf{V}^{\ell}$ is a trainable MLP.

Virtual Nodes enable global information exchange after each layer.

Local Tasks on Massive Graphs

Dataset: One huge graph with billions of vertices.

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Sampling Algorithms:

- GraphSAGE [Hamilton et al., 2017]
- HGSampler [Hu et al., 2020]

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This is an active field of research.

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- Implement global pooling with scatter operations.
- Implement a Virtual Node layer.
- Evaluate your implementation on the ZINC dataset.

References I

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