

Setup Instructions:

1. Navigate to https://github.com/GageDeZoort/prc_gnn_tutorial
2. Click on gnn_tutorial_3_27_23.ipynb
3. Change “github” to “githubtocolab” in your searchbar, i.e.:
https://colab.research.google.com/github/GageDeZoort/prc_gnn_tutorial
4. If you want to use a GPU (none of the cells require one), you can request one on Colab through Edit->Notebook Settings

The background features a complex network diagram with various sized nodes (circles) in dark blue, light blue, and grey, connected by thin grey lines. Some nodes are highlighted with larger concentric circles. A dark grey rectangular box is positioned in the lower right quadrant, containing white text.

GRAPH NEURAL NETWORKS

PICSCIE/RESEARCH COMPUTING

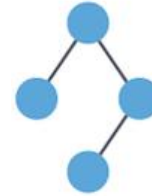
Gage DeZoort

3/27/23

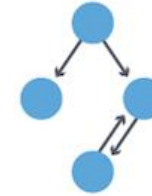
GRAPHS

- Graphs represent relational data
 - Entities \rightarrow Nodes: $u \in \mathcal{V}$
 - Node features: $\mathbf{x}_u \in \mathbb{R}^{d_v}$
 - Relations \rightarrow Edges: $(u, v) \in \mathcal{E}$
 - Edge features: $\mathbf{e}_{uv} \in \mathbb{R}^{d_e}$

Undirected

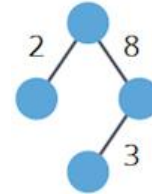


Directed

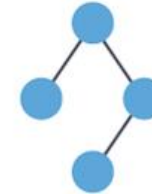


Directed edges specify an incoming and outgoing node

Weighted

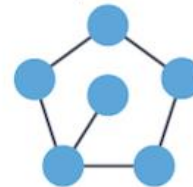


Unweighted



Edge features might be weights or otherwise more complicated attributes

Sparse



Dense



Sparsity is problem-dependent... roughly, sparse if $|\mathcal{E}| \ll |\mathcal{V}|^2$

EDGE REPRESENTATIONS

- Graphs represent relational data
 - Entities \rightarrow Nodes: $u \in \mathcal{V}$
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 - Relations \rightarrow Edges: $(u, v) \in \mathcal{E}$
 - Edge features: $\mathbf{e}_{uv} \in \mathbb{R}^{d_e}$

Edge Representations

Adjacency Matrices

$$A_{adjacency} \in \mathbb{R}^{d_v \times d_v}$$

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Incidence Matrices

$$A_{incidence} \in \mathbb{R}^{d_v \times d_e}$$

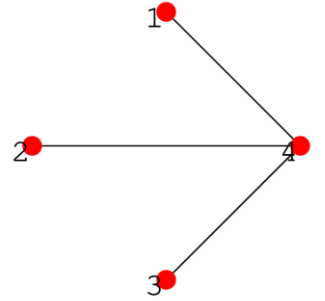
$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$



Sparse Index Lists (COO)

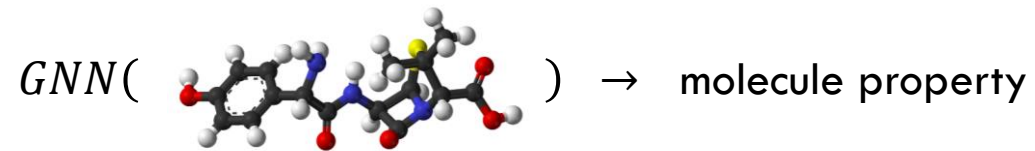
$$I_{COO} \in \mathbb{R}^{2 \times d_e}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 4 & 4 \end{bmatrix}$$

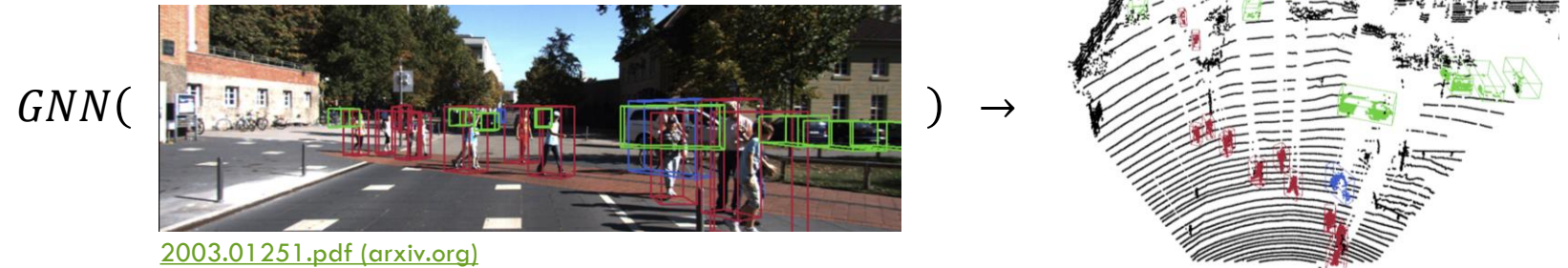


GRAPH LEARNING TASKS

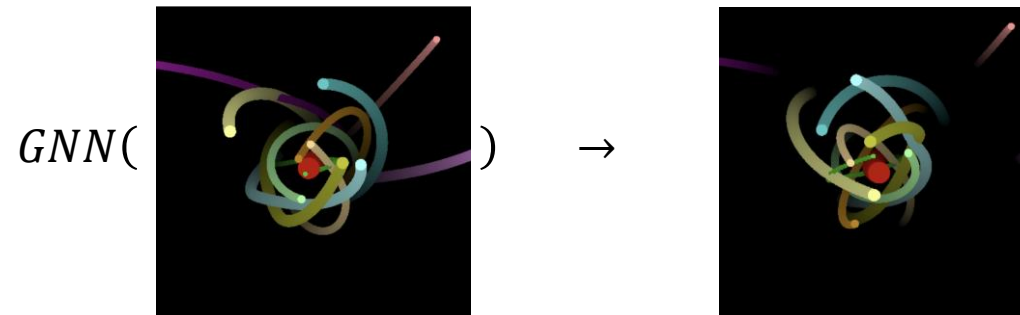
DRUG DISCOVERY



INSTANCE SEGMENTATION

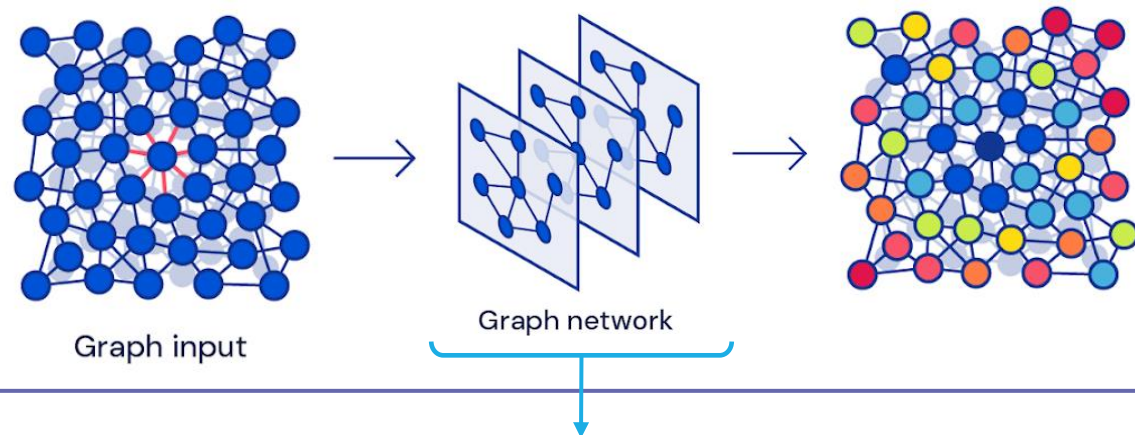


PHYSICS SIMULATION

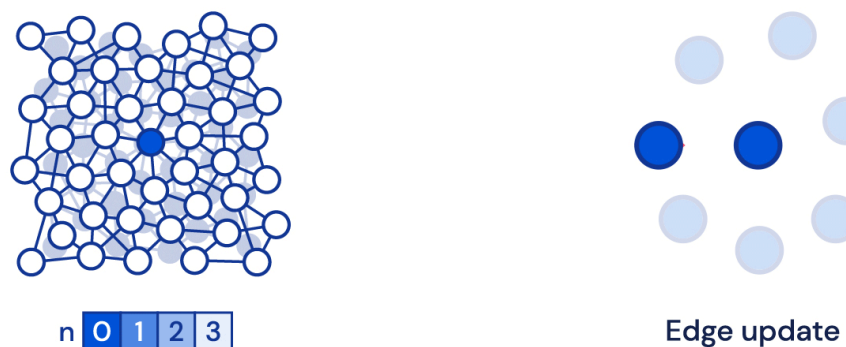


[\[1612.00222\] Interaction Networks for Learning about Objects, Relations and Physics \(arxiv.org\)](#)

GNNs: High-Level View

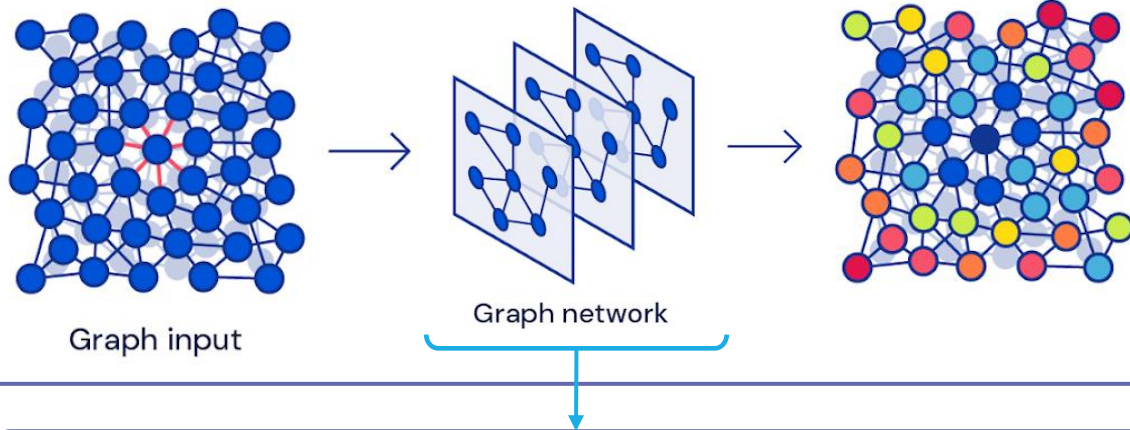


GNN Layers, Neural Message Passing

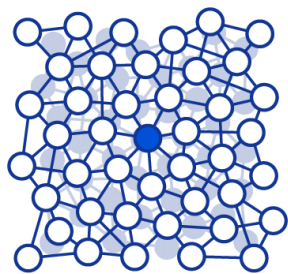


“Messages” computed from each node’s neighborhood are used to update graph features... k iterations \rightarrow info from k -hop neighborhood

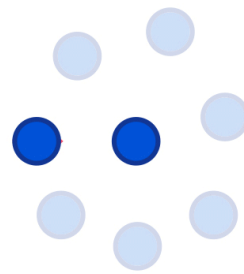
GNNs: High-Level View



GNN Layers, Neural Message Passing



n 0 1 2 3



Edge update

“Messages” computed from each node’s neighborhood are used to update graph features... k iterations \rightarrow info from k -hop neighborhood

Message Passing (MPNN) Layers:

Framework for many equivariant graph updates

At each layer k , compute messages in each node’s neighborhood:

$$\mathbf{m}_{uv}^{(k)} = \psi^{(k)} \left(\mathbf{h}_u^{(k-1)}, \mathbf{h}_v^{(k-1)}, \mathbf{e}_{uv}^{(k-1)} \right)$$

Aggregate messages in a permutation-invariant way:

$$\mathbf{a}_u^{(k)} = \bigoplus_{v \in N(u)} \mathbf{m}_{uv}^{(k)}$$

Messages passed only from u ’s direct neighbors

Any permutation invariant operation (e.g. sum, mean, max)

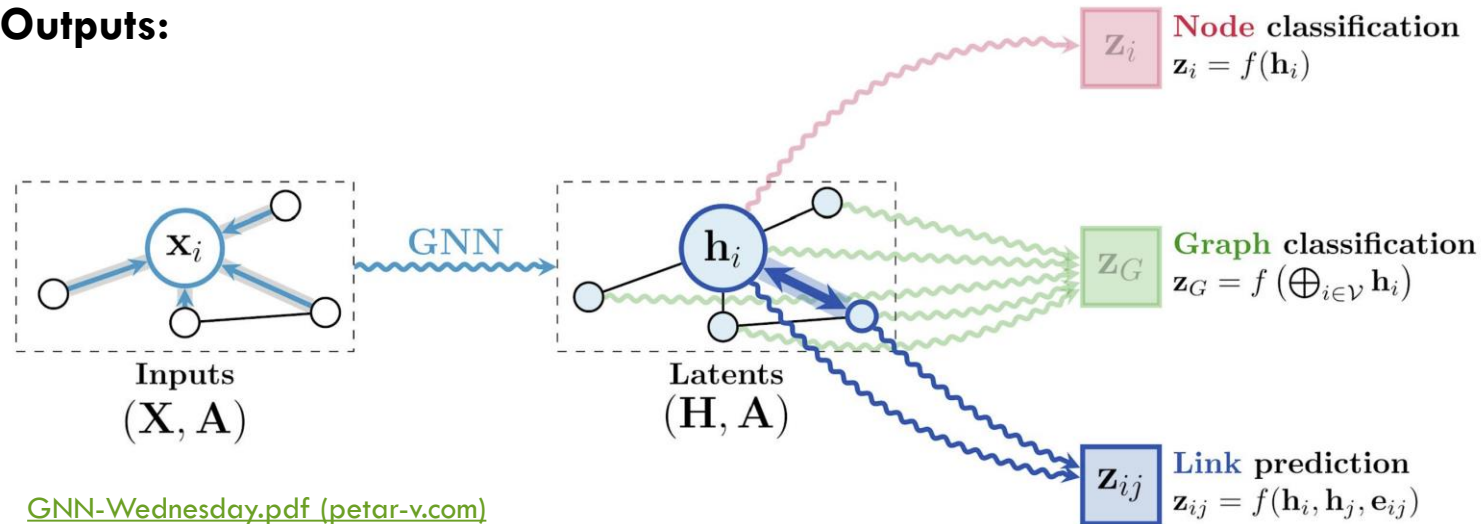
Update the node’s state based on the messages it received:

$$\mathbf{h}_u^{(k)} = \phi^{(k)} \left(\mathbf{h}_u^{(k-1)}, \mathbf{a}_u^{(k)} \right)$$

Generic MPNN Layers:

$$\mathbf{h}_u^{(k)} = \phi^{(k)} \left[\mathbf{h}_u^{(k-1)}, \bigoplus_{v \in N(u)} \psi^{(k)} \left(\mathbf{h}_u^{(k-1)}, \mathbf{h}_v^{(k-1)}, \mathbf{e}_{uv}^{(k-1)} \right) \right]$$

Outputs:





Tutorial Agenda

0. Software Setup

1. Graph-Structured Data
 1. Karate Club (node classification)
 2. ENZYMES (graph classification)
2. Graph Neural Networks
 1. GCN Math
 2. Training on Cora
3. Long Exercise: graph-level training with ENZYMES (Optional)
4. Message Passing Under the Hood (Optional)