Seminar Series on Graph Neural Networks 01

# Introduction to Graph Mining and Graph Neural Networks

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# Before going in....

Wrap-up: Message passing all the way up
(Up-to-date comprehensive survey on GNN archtiectures)

**Towards application of graph neural networks**

Towards efficient graph learning

Explainable graph neural networks

**Fundamental topics on graph neural networks**

On the representational power of graph neural networks

A graph signal processing viewpoint of graph neural networks

On the problem of oversmoothing and oversquashing

Introduction to graph mining and graph neural networks
(Current session, basic overview to kick things off)

**(Some of the topics may change in the future for a better alternative)**

* Presentation slides are available at:
(jordan7186.github.io/presentations/)

# Objectives

1. Understanding of **graphs** as a **general data type**
2. Understanding of the general framework of **graph neural networks (GNNs)**
3. High-level understanding of **several key GNN architectures: GCN & GraphSAGE**

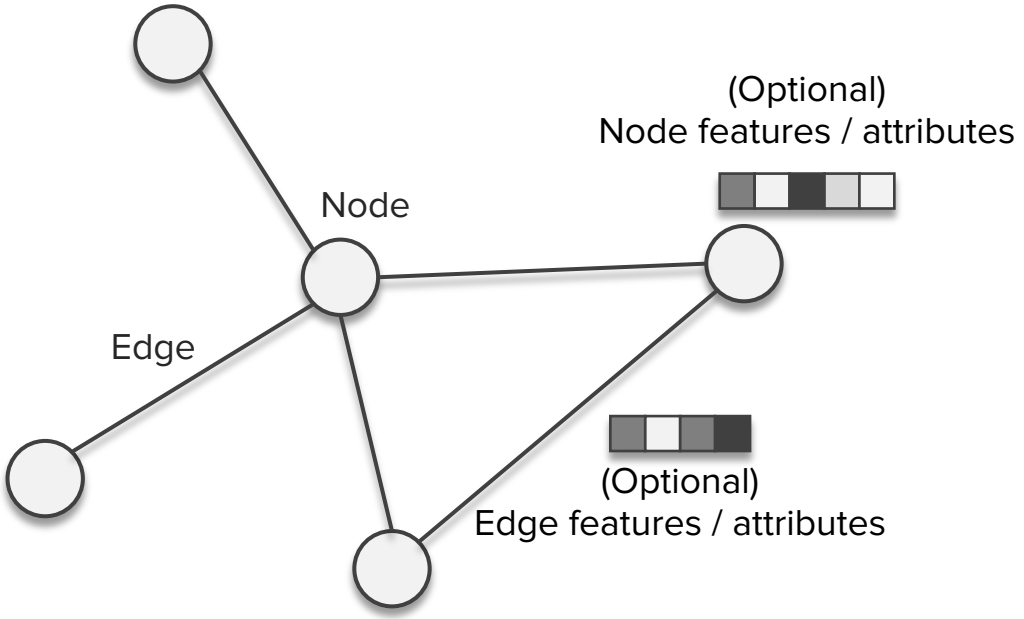
# Understanding of graphs as a general data type

*This part is heavily influenced by one of my academic heros, Petar Veličković. These are some materials from his public materials that I have referred to:

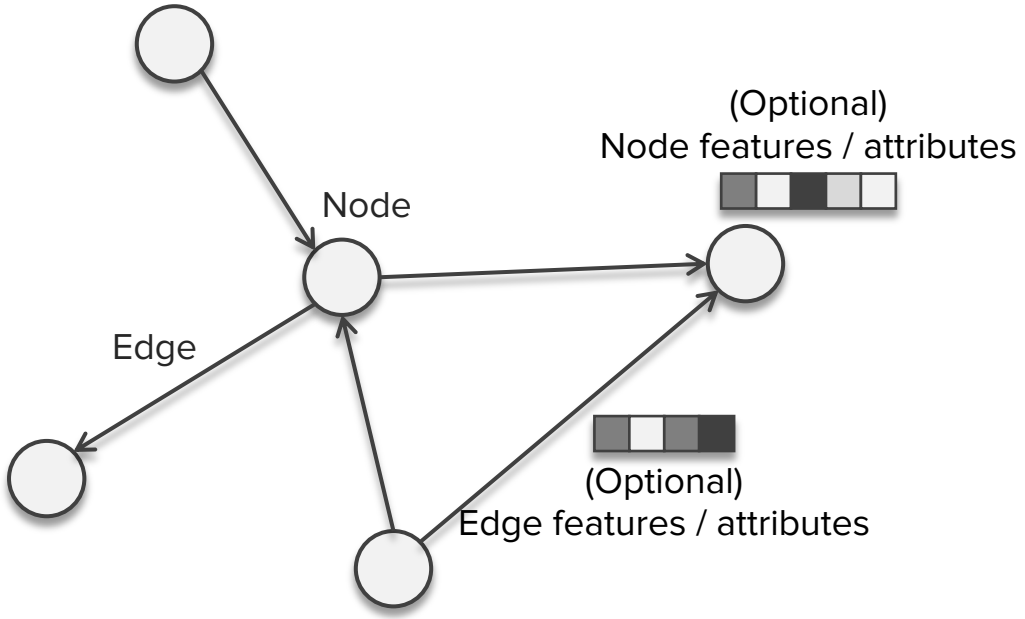
- (Slide) Everything is Connected: Graph Neural Networks from the Ground Up (2021)
- (Blog) Graph & Geometric ML in 2024: Where We Are and What's Next (Part II – Applications)

# Graphs as an abstract datatype

Graphs are an abstract type of data where nodes (entities) are **connected** by edges (connections)




Undirected graph




Directed graph

...But honestly, looking at this does not result in a **practical** understanding of graphs.

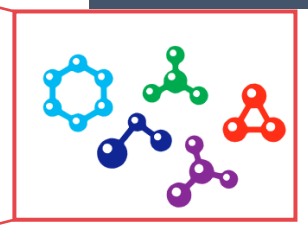
Therefore, we will look at **various applications** in the field of **graph machine learning** before moving our discussion further.

# Area 1) Biology & Chemistry Research

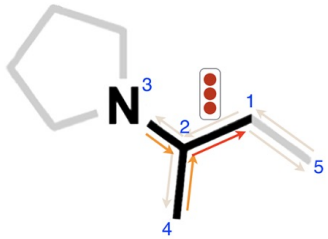
## Example 1: The discovery of Halicin, GNN-guided antibiotic discovery

Node: Atom
Edge: Atom bonds
Edge feature: Bond type etc.

**Training GNNs with real-world chemical dataset**



Training set
($10^4$ molecules)




**Prediction task**
*E.coli growth inhibition*

Apply

**Drug dataset (~6K)**

Acquire potential lead compounds that acts a gainst E.coli

Further screening & Empirical testing

Cell

Article

**A Deep Learning Approach to Antibiotic Discovery**

Jonathan M. Stokes,[1,2,3] Kevin Yang,[3,4,10] Kyle Swanson,[3,4,10] Wengong Jin,[3,4] Andres Cubillos-Ruiz,[1,2,5] Nina M. Donghia,[1,9] Craig R. MacNair,[6] Shawn French,[6] Lindsey A. Carfrae,[6] Zohar Bloom-Ackermann,[2,7] Victoria M. Tran,[2] Anush Chiappino-Pepe,[5,7] Ahmed H. Badran,[2] Ian W. Andrews,[1,2,5] Emma J. Chory,[1,2] George M. Church,[5,7,8] Eric D. Brown,[6] Tommi S. Jaakkola,[3,4] Regina Barzilay,[3,4,9,*] and James J. Collins[1,2,5,8,9,11,*]

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[4]Computer Science and Artificial Intelligence Laboratory, Massachusetts Institute of Technology, Cambridge, MA 02139, USA
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[7]Department of Genetics, Harvard Medical School, Boston, MA 02115, USA
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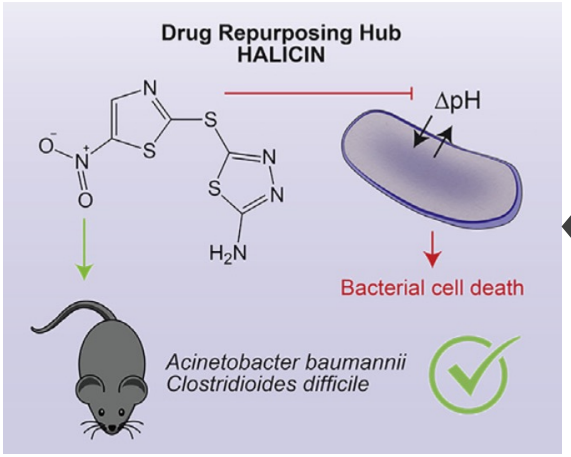
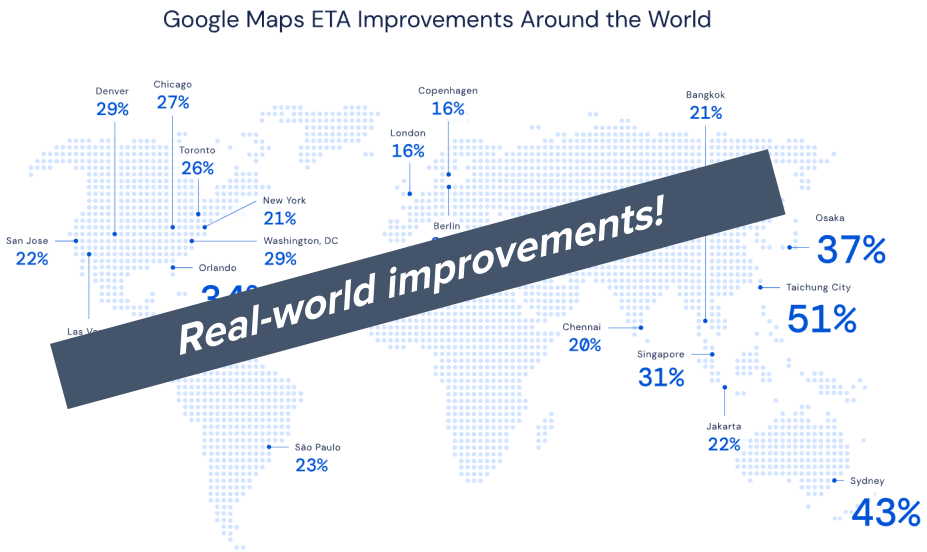
*Correspondence: regina@csail.mit.edu (R.B.), jimjc@mit.edu (J.J.C.)
https://doi.org/10.1016/j.cell.2020.01.021

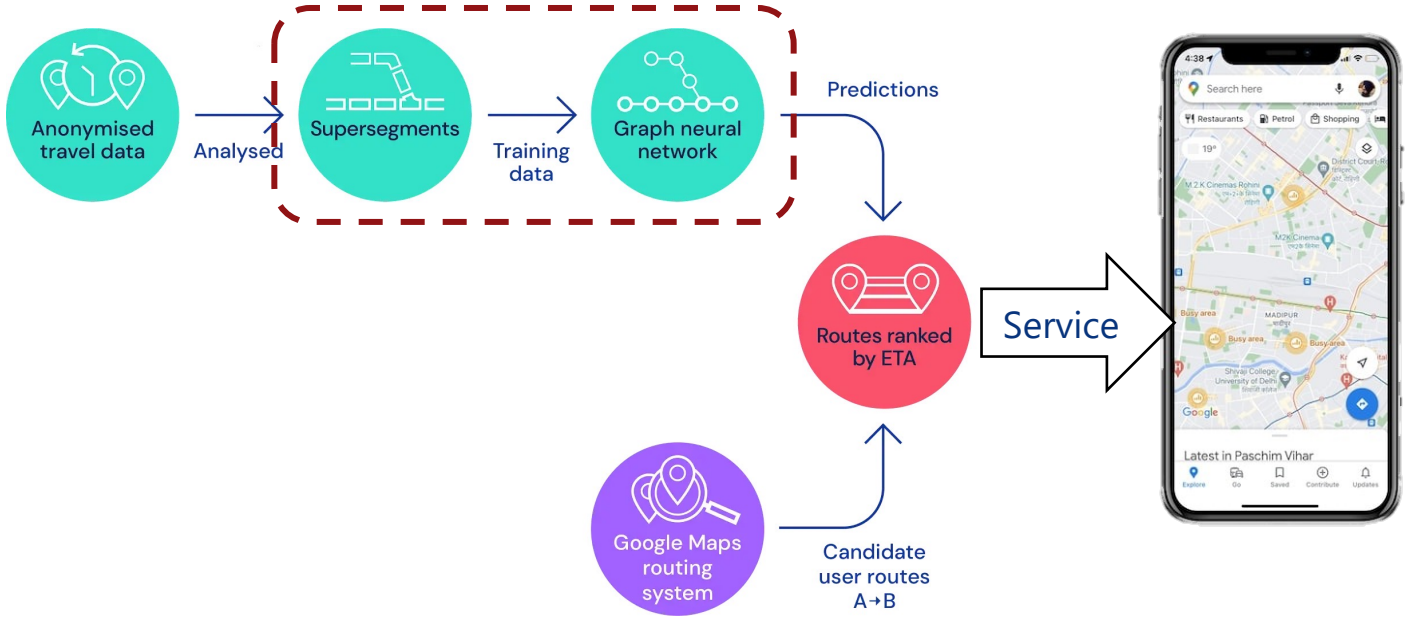



Stokes, Jonathan M., et al. "A deep learning approach to antibiotic discovery." Cell 180.4 (2020): 688-702.
Yang, Kevin, et al. "Analyzing learned molecular representations for property prediction." Journal of chemical information and modeling 59.8 (2019): 3370-3388.

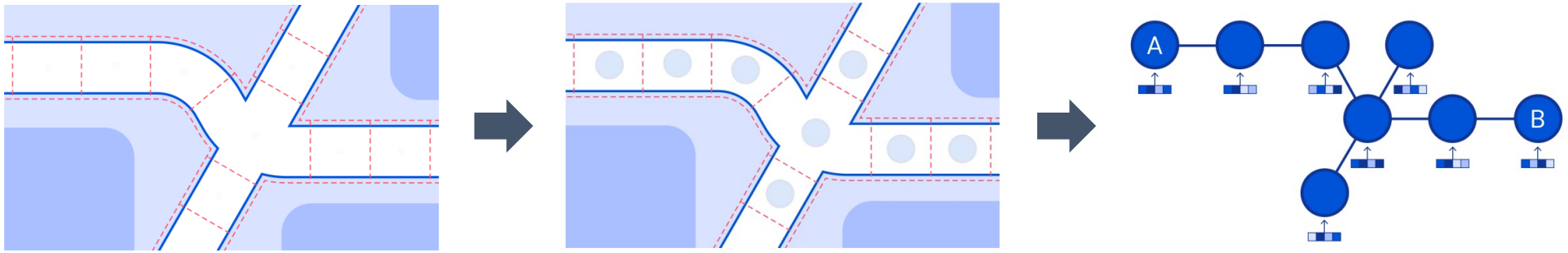
# Area 2) ETA prediction

## Example 2: DeepMind's improvement of Google map's ETA (Estimated Time of Arrival) prediction




Unlike chemical datasets, constructing a graph is less straightforward.
In these cases, **how to construct the graph** is also a crucial contribution.

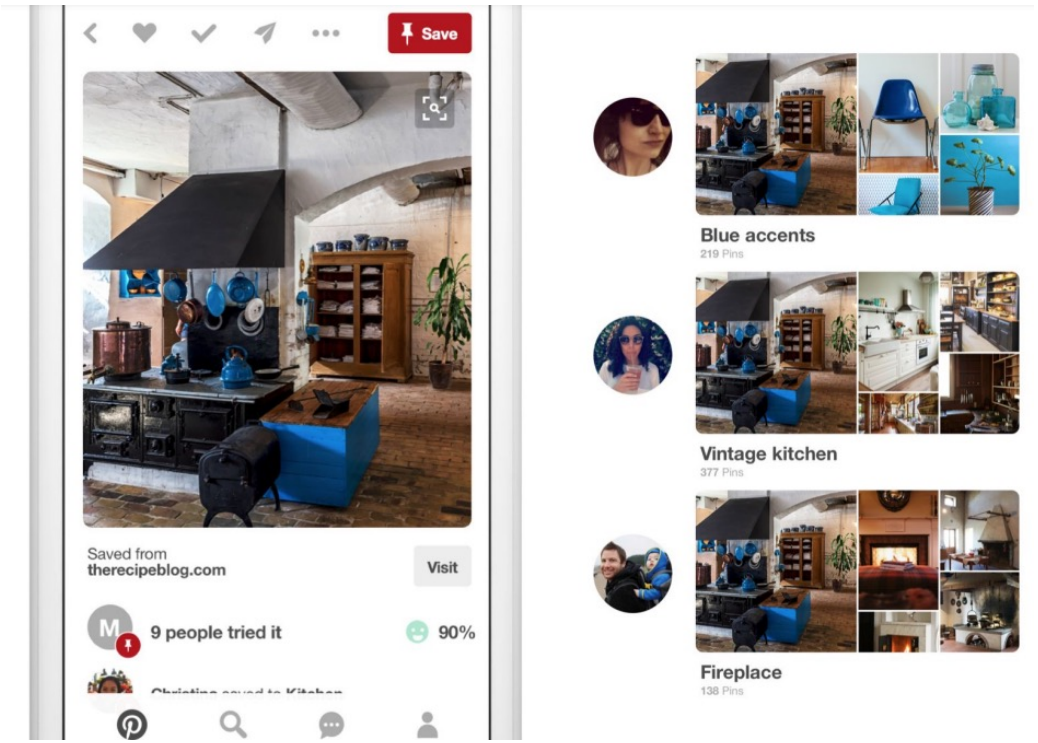



Derrow-Pinion, Austin, et al. "ETA prediction with graph neural networks in google maps.", CIKM 2021.
Deepmind, "Traffic prediction with advanced graph neural networks"

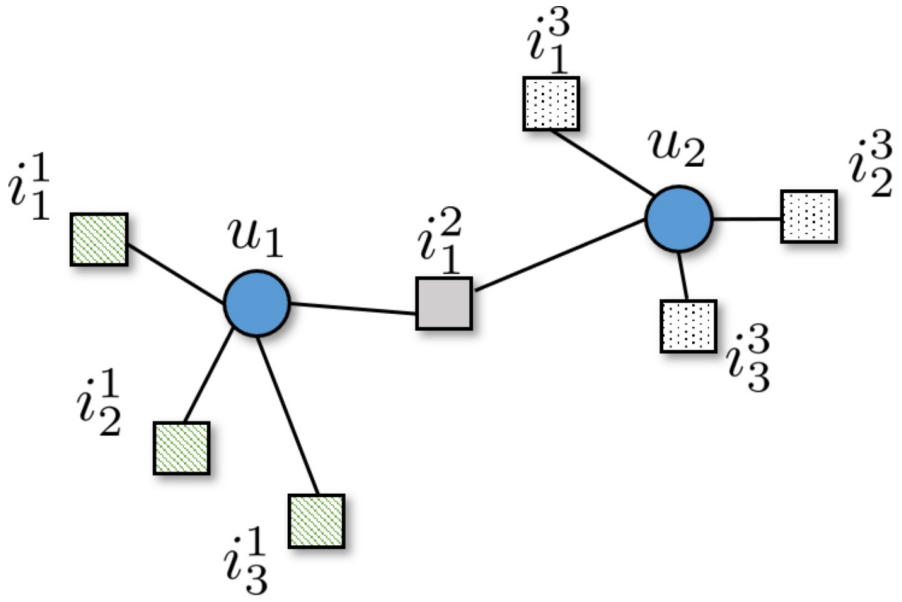
# Area 3) Recommdender systems

## Example 3: Pinterest (social platform)

### Image & User interaction in Pinterest



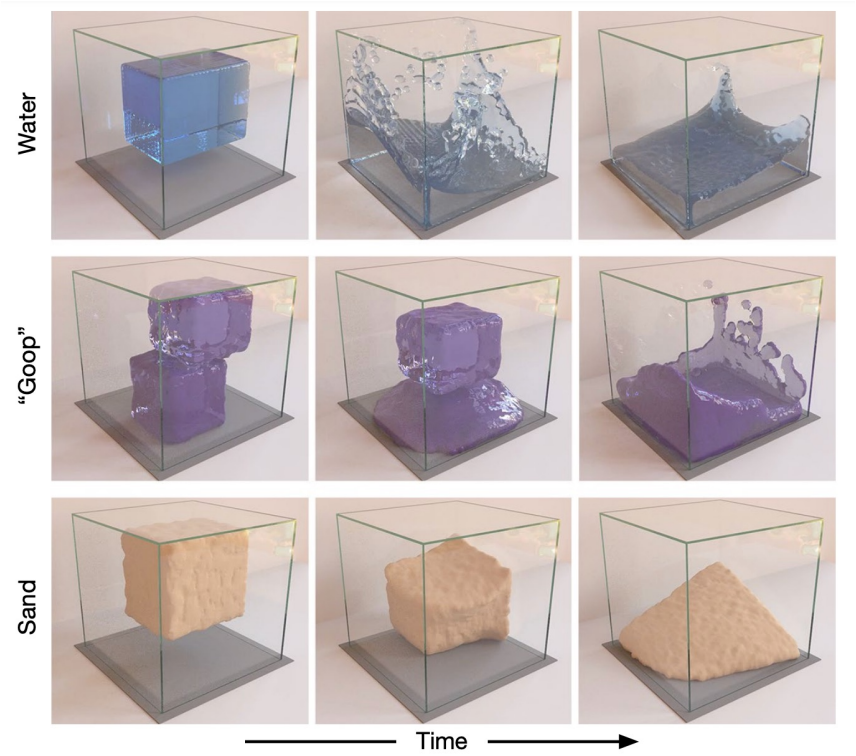

### User-item interaction graph

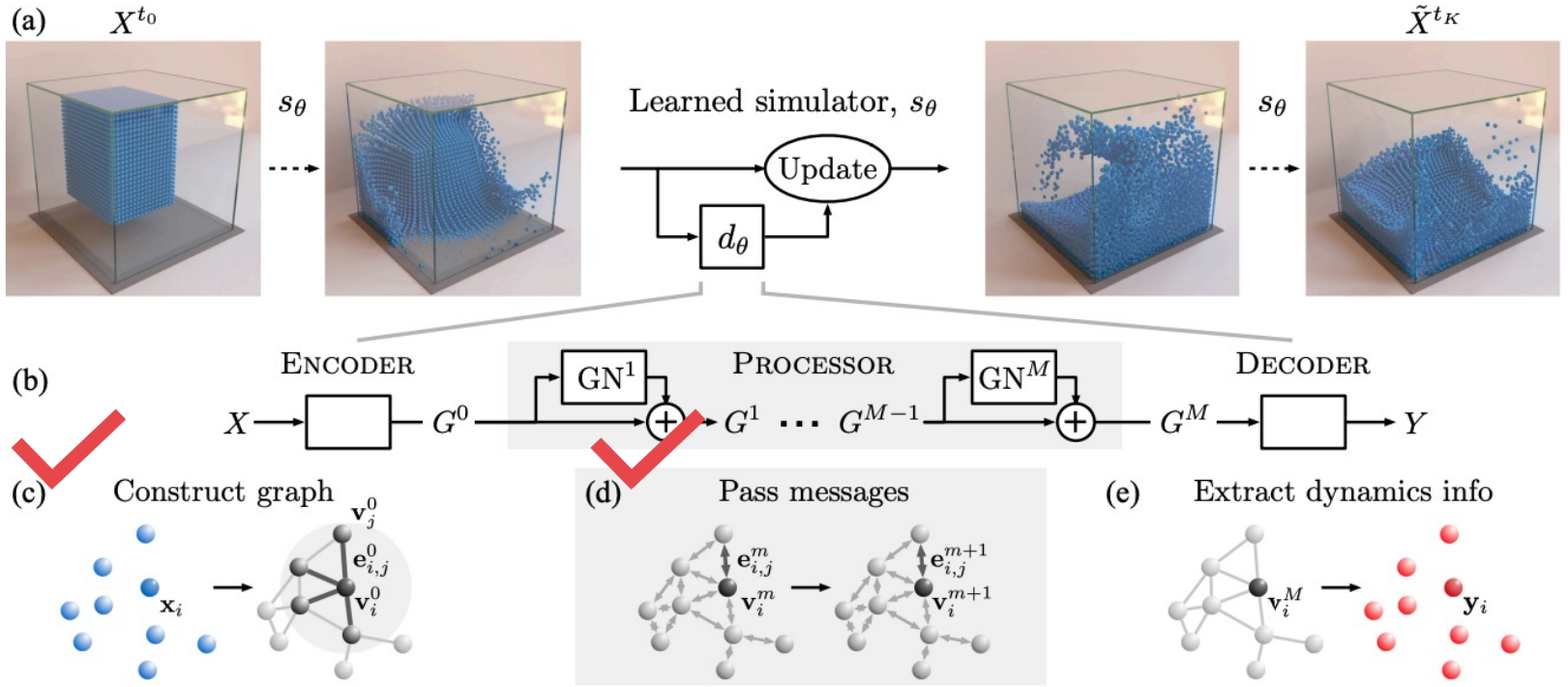



Source: Andrew Zhai (Pinterest) talk @WWW 2022 (link)
Right figure: Hou et al., Collaborative Filtering Based on Diffusion Models: Unveiling the Potential of High-Order Connectivity, SIGIR 2024

# Area 4) Modeling physical systems

## Example 4: Simulation of complex physical systems



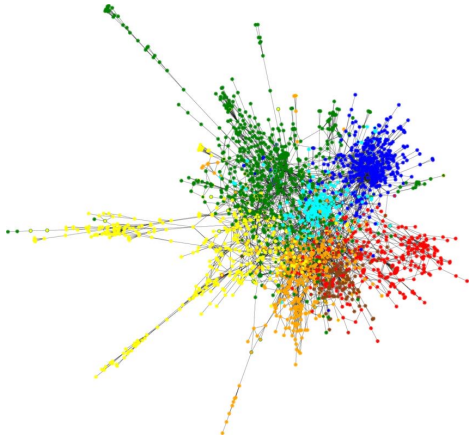

Sanchez-Gonzalez et al., Learning to Simulate Complex Physics with Graph Networks, ICML 2020

# In academia: Benchmark datasets in the literature

## Social

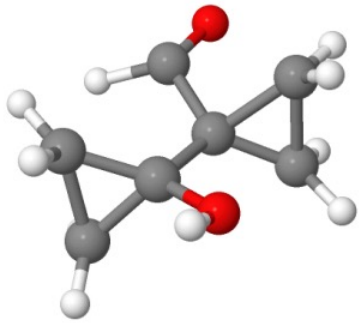
Node: People / Account
Edge: Connection
Node feature: Metadata

## Citation / Web



Node: Paper
Edge: Citation
Node feature: Abstract

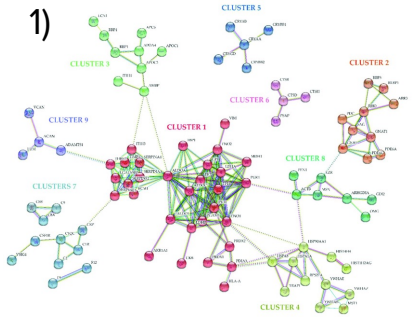
## Molecules



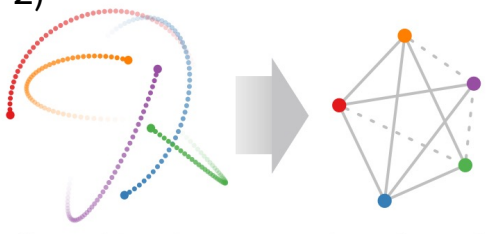
Node: Atom
Edge: Bond
Node feature: Atom type
Edge feature: Bond type

## Biology / Simulation / etc.

1)

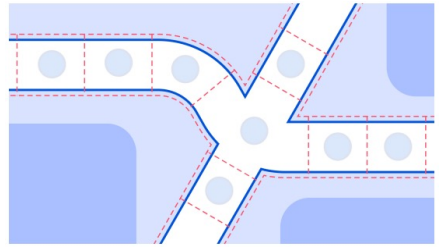


2)




3)

4)



### Example benchmark datasets

- Reddit
- Ego-Facebook
- Github

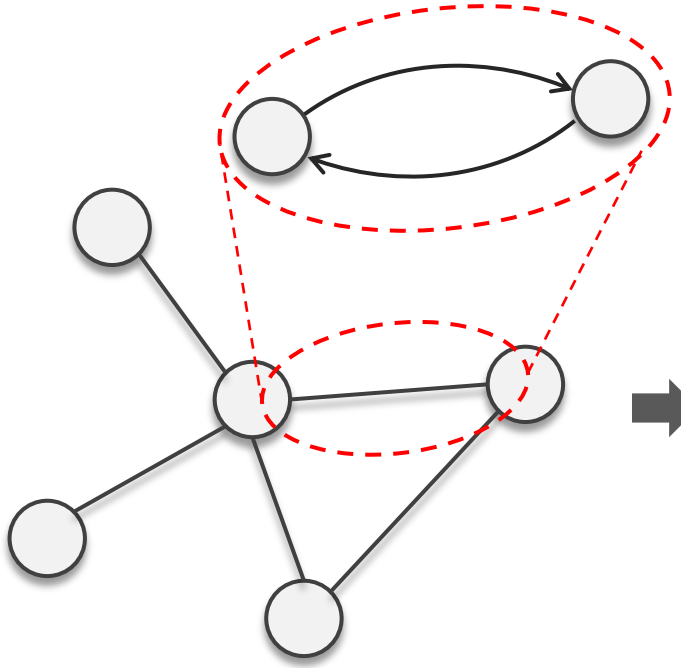
- *Planetoid dataset (Cora/Citeseer/Pubmed)
- Coauthor
- WebKB (Texas/Cornell/etc.)

- QM9
- Zinc
- MUTAG

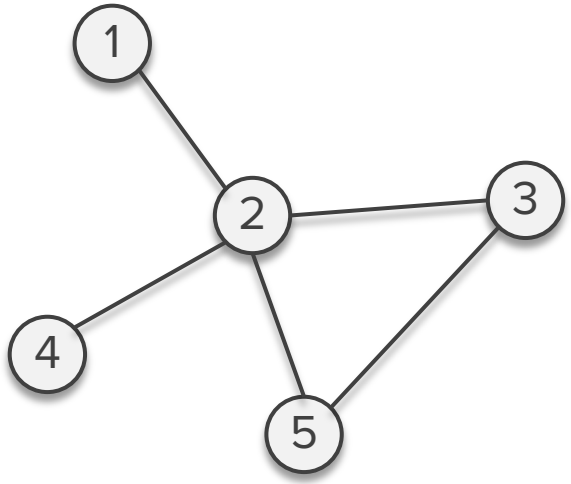
1) **PPI (protein-protein interaction)
2) Physical simulation (Kipf et al., 2018)
3) 3D point cloud (Wang et al., 2019)
4) Road network (Derrow-Pinion et al., 2021)

Yang et al., Revisiting Semi-Supervised Learning with Graph Embeddings, ICML 2016
Kipf et al., Neural Relational Inference for Interacting Systems, ICML 2018
Wang et al., Dynamic Graph CNN for Learning on Point Clouds, ACM Transactions on Graphics 2019
Derrow-Pinion et al., ETA Prediction with Graph Neural Networks in Google Maps, CIKM 2021
**Image source: https://www.researchgate.net/publication/324457787_iTRAQ_Quantitative_Proteomic_Analysis_of_Vitreous_from_Patients_with_Retinal_Detachment/figures?lo=1

# Representing the graph as a adjacency matrix



*We treat undirected edges as
two directed edges going in both directions




| | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 1 | 0 | 1 | 0 | 0 | 0 |
| 2 | 1 | 0 | 1 | 1 | 1 |
| 3 | 0 | 1 | 0 | 0 | 1 |
| 4 | 0 | 1 | 0 | 0 | 0 |
| 5 | 0 | 1 | 0 | 1 | 0 |

**Undirected graph**

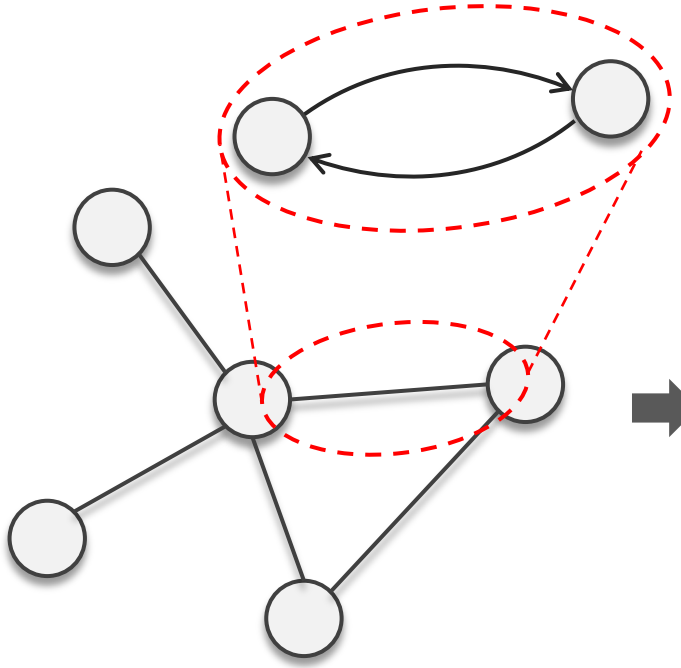
**Assign arbitrary node ordering**

- **Graphs with canonical node ordering is not common**
- Related research topic: Positional encoding of nodes
  (As an example, see [1] )

**Adjacency matrix**

- Represent edge by assigning 1 for (i, j)-th element if node i and j are connected
- For weighted graphs: Assign a real number
- For graphs with multiple edges: Assign integers
- For directed graphs: Asymmetric matrix

# Representing the graph as a adjacency matrix



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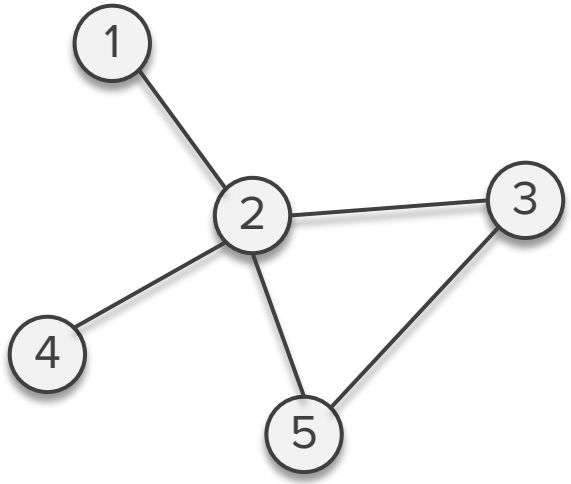



(1, 2), (2, 1), (2, 3), (3, 2), …

**Undirected graph**

**Assign <u>arbitrary</u> node ordering**

- **Graphs with canonical node ordering is not common**
- Related research topic: Positional encoding of nodes
  (As an example, see [1] )

**Edge list**

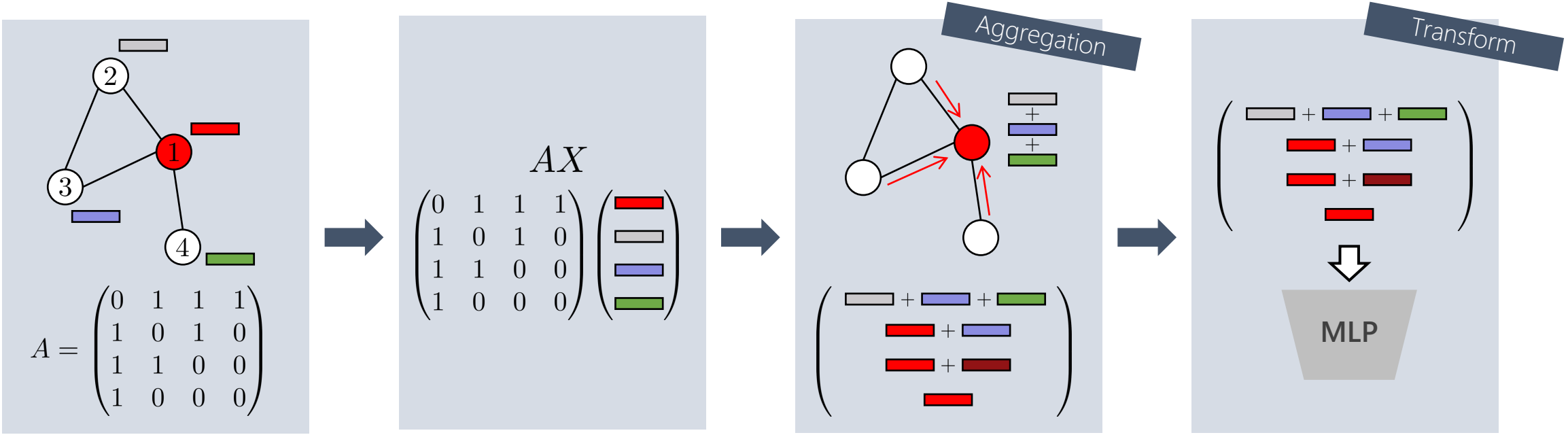
- Represent graph by listing all edges
- Notice that for undirected edges, (i, j) and (j,i) both appear
- More **memory efficient** than (dense) adjacency matrix

# Understanding of the general framework of graph neural networks (GNNs)

# A simple, popular, and straightforward GNN

GCN (Graph Convolutional Network): Kipf & Welling, ICLR 2017

**We are now ready to understand the basic principles of GNN, by looking at the most popular architecture.**




Notice that, this whole procedure can be neatly expressed as: $\sigma(AX\Theta)$

Of course, all of this still holds **when we scramble the node ordering** (permutation invariant)

Non-linear activation function $\sigma(\cdot)$

Adjacency matrix $A \in \mathbb{R}^{n \times n}$

Node feature matrix $X \in \mathbb{R}^{n \times d}$

Learnable matrix $\Theta \in \mathbb{R}^{d \times d'}$

n: # of nodes

d: node feature dimensions

d': dimension for the next layer

# A simple, popular, and straightforward GNN

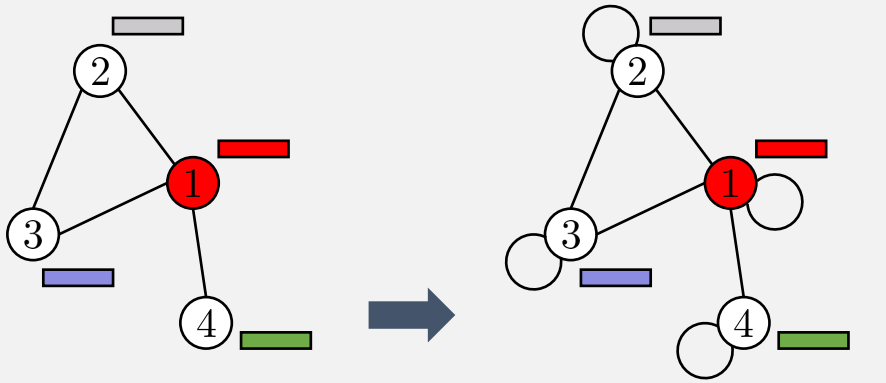
GCN (Graph Convolutional Network): Kipf & Welling, ICLR 2017

**Of course, we can get creative with the graph structure to solve some practical issues**

Problem 1: The information of the neighbor nodes are aggregated but not the node itself.
Problem 2: The adjacency matrix is not normalized, and the scale of the feature vectors may explode for repeated layers.

## Resolution to problem 1

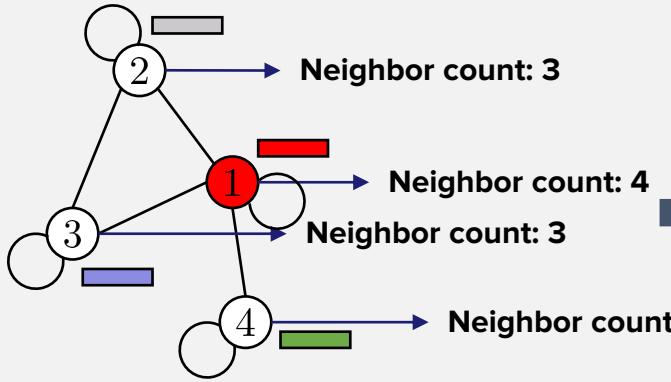
Add self-loops to each node




$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \hat{A} = A + I = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

## Resolution to problem 2

Normalization of $\hat{A}$:




$$D = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

$$\tilde{A} = \hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2} = \begin{pmatrix} \frac{1}{4} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{12}} & \frac{1}{\sqrt{8}} \\ \frac{1}{\sqrt{12}} & \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{\sqrt{12}} & \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{1}{\sqrt{8}} & 0 & 0 & \frac{1}{2} \end{pmatrix}$$

Final layer of GCN: $\sigma(\tilde{A}X\Theta)$

# Abstraction: A general message-passing layer of GNNs

**1. Message passing phase (Aggregation)**

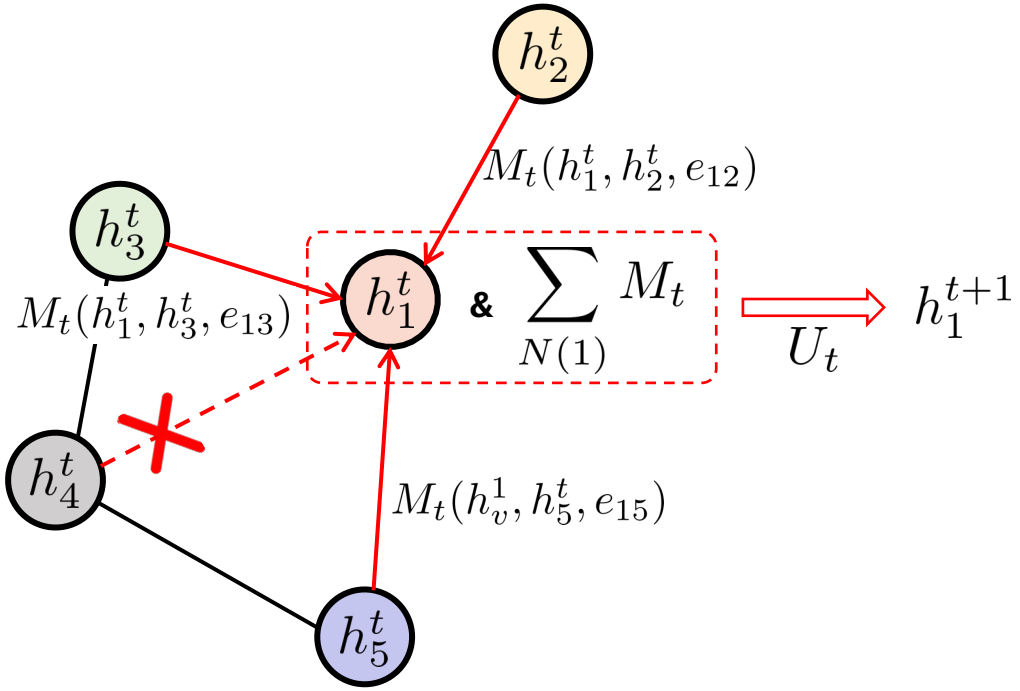
$$m_v^{t+1} = \sum_{w \in N(v)} M_t(h_v^t, h_w^t, e_{vw})$$

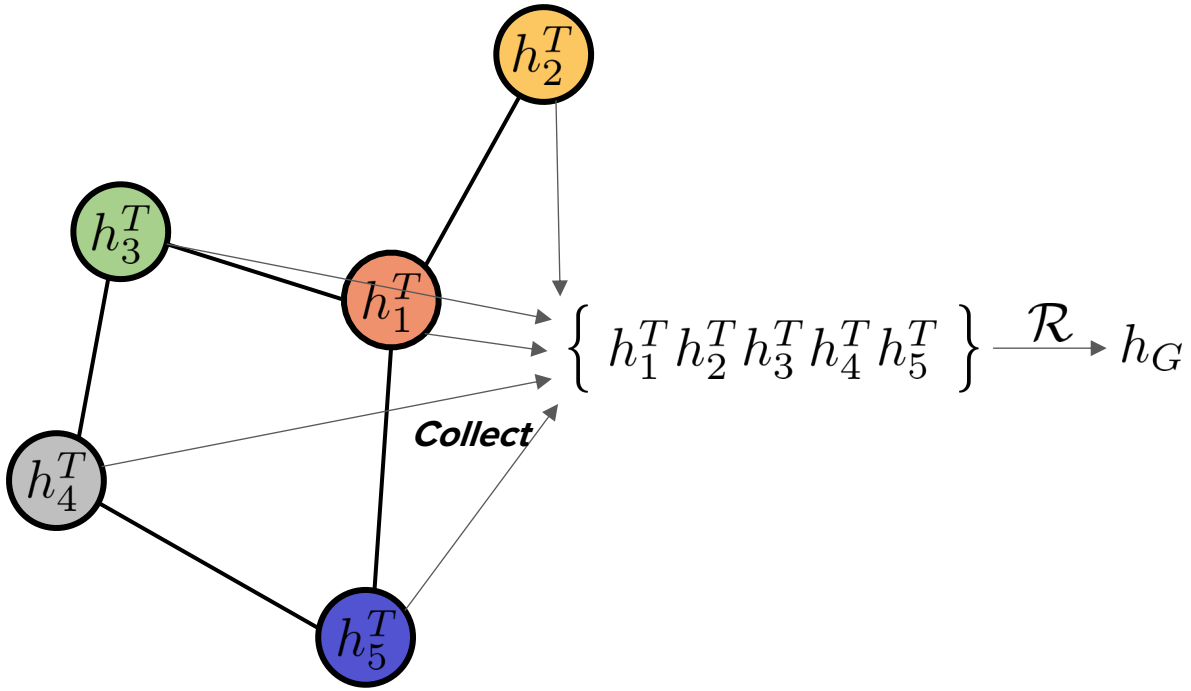
**2. Update phase (Transformation)**

$$h_v^{t+1} = U_t(h_v^t, m_v^{t+1})$$

**3. Readout phase (Only for graph-level tasks)**

$$h_G = \mathcal{R}(h_1^T, \cdots, h_{\mathcal{V}}^T)$$



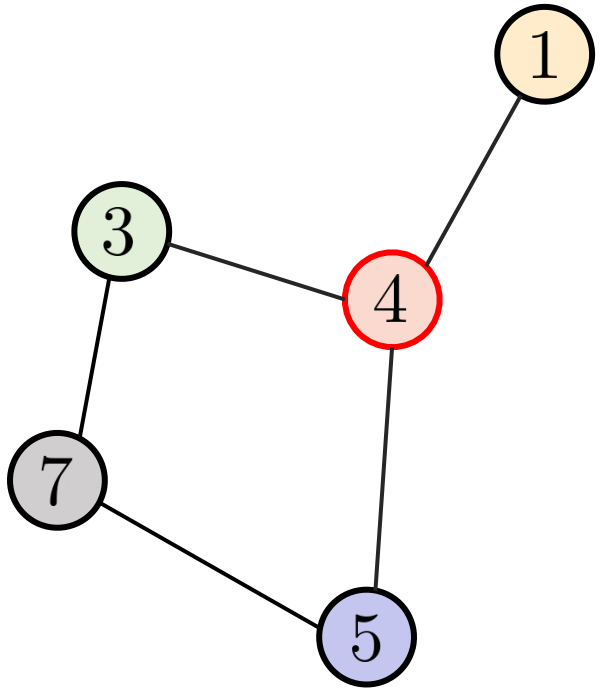




*Usually, we cite these papers for the term “message-passing”

[First formal introduction of the concept] Gilmer et al., “Neural Message Passing for Quantum Chemistry”, ICML 2017
[Comprehensive discussion & abstraction] Bronstein et al., Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges, arXiv 2021

# Abstraction: A general message-passing layer of GNNs

## GNN layer (Message-passing neural networks)




$$\mathbf{h}_u = \phi\left(\mathbf{x}_u, \bigoplus_{v \in \mathcal{N}_u} \psi(\mathbf{x}_u, \mathbf{x}_v)\right)$$

$\bigoplus$

This operation must be permutation invariant to ensure the same result for different node orderings!
**Summation / Average / Max pooling** etc.

So if we re-describe GCN for node 4, it would be...

$$\mathcal{N}_u = \{1, 3, 5\} \cup \{4\} \quad \psi(\mathbf{x}_u, \mathbf{x}_1) = \frac{1}{\sqrt{2 \times 4}}\mathbf{x}_1 \quad \phi = \text{MLP}$$

*Usually, we cite these papers for the term “message-passing”
[First formal introduction of the concept] Gilmer et al., “Neural Message Passing for Quantum Chemistry”, ICML 2017
[Comprehensive discussion & abstraction] Bronstein et al., Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges, arXiv 2021

## High-level understanding of several key GNN architectures

# A list of noteworthy GNN architectures



## Frequently used architectures (Must know!)

**GCN)** Kipf & Welling, “Semi-supervised classification with graph convolutional networks”, ICLR 2017

**GraphSAGE)** Hamilton et al., “Inductive representation learning on large graphs”, NeurIPS 2017

**GAT)** Veličković et al., “Graph attention networks”, ICLR 2018

**GIN)** Xu et al., “How powerful are graph neural networks?”, ICLR 2019 (we will come back to this in later seminars)

## Lightweight GNNs (we will come back to this in later seminars)

**SGC)** Wu et al., “Simplifying graph convolutional networks”, ICML 2019

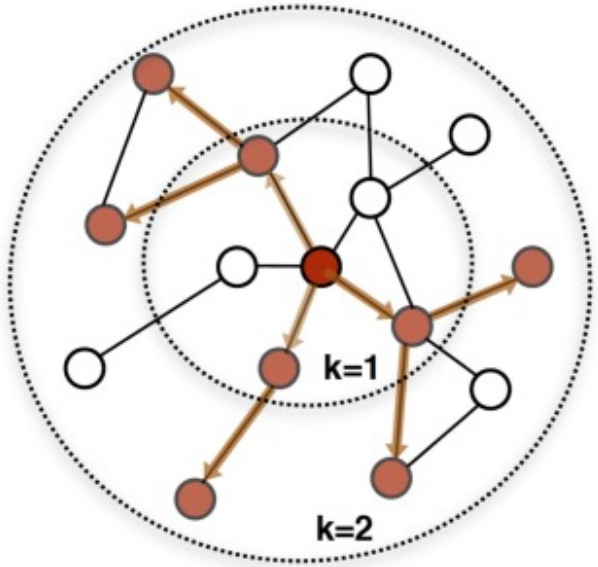
**LightGCN)** He et al., “LightGCN: Simplifying and powering graph convolutional network for recommendation, SIGIR 2020

## Spectral viewpoint of GNNs (we will come back to this in later seminars)

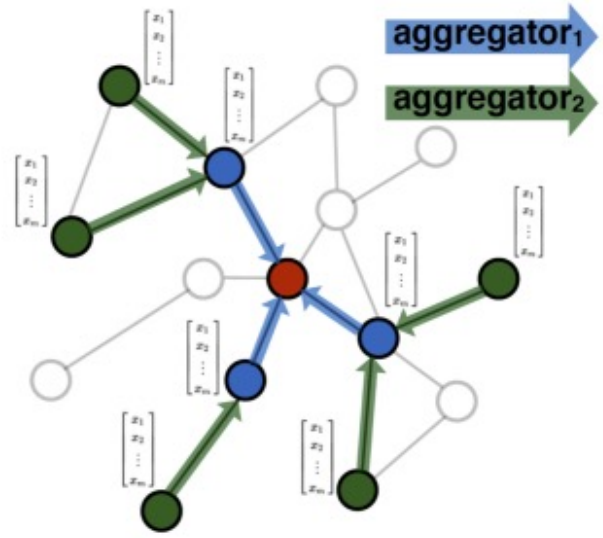
**ChebNet)** Defferrard et al., “Convolutional neural networks on graphs with fast localized spectral filtering”, NeurIPS 2016

# GraphSAGE: Introduction of neighbor sampling

**Problem**: As we stack multiple layers, we introduce a **LOT** of neighboring nodes during message-passing.




1. Sample neighborhood



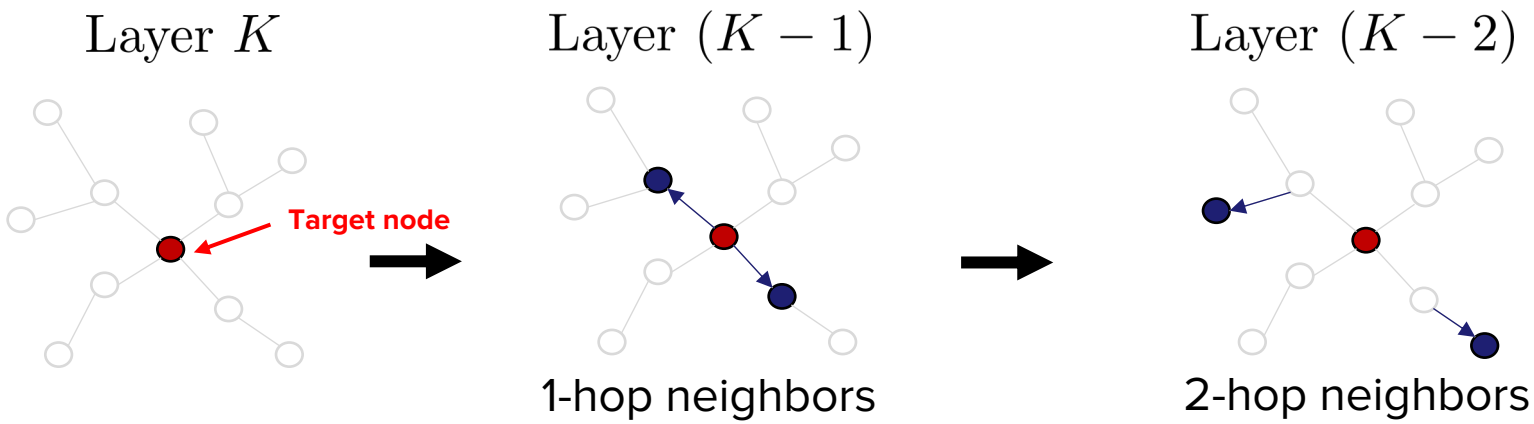

2. Aggregate feature information from neighbors

Sampling the neighbor nodes (contrast to using all neighbors) reduce memory complexity and still achieves good performance.

*In my experience, these type of intuitions (trading off speed and/or memory by dropping some nodes/edges) work better for social graph types

# GraphSAGE: Introduction of neighbor sampling

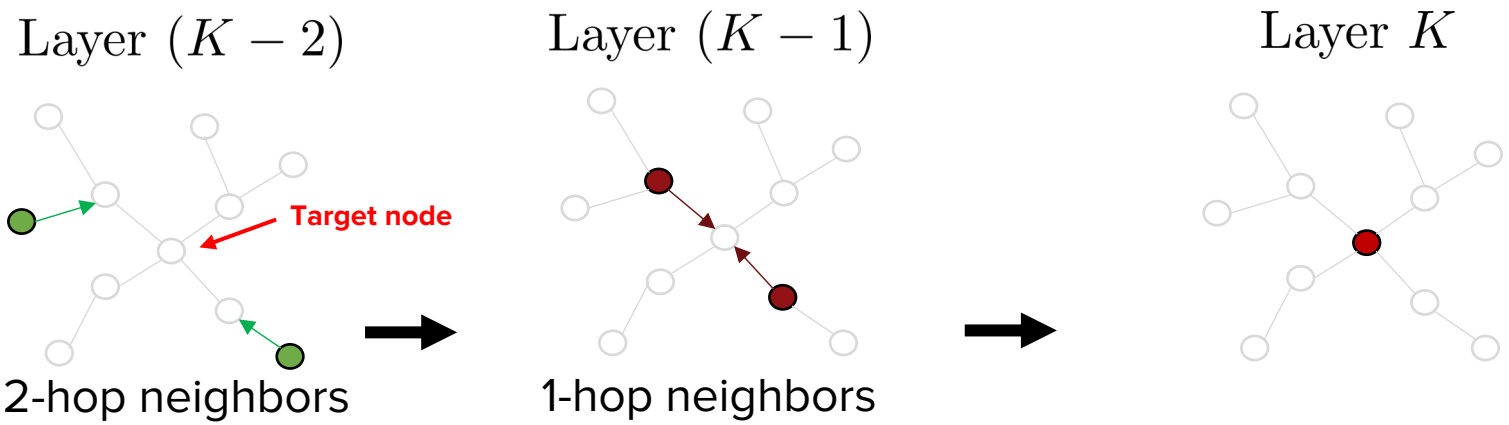
$\mathcal{B}^K \leftarrow \mathcal{B}$;
**for** $k = K...1$ **do**
  $B^{k-1} \leftarrow \mathcal{B}^k$ ;
  **for** $u \in \mathcal{B}^k$ **do**
    $\mathcal{B}^{k-1} \leftarrow \mathcal{B}^{k-1} \cup \mathcal{N}_k(u)$;
  **end**
**end**




The sampling process is conceptually reversed compared to forward pass.

# GraphSAGE: Introduction of neighbor sampling

**for** $k = 1...K$ **do**
  **for** $u \in \mathcal{B}^k$ **do**
    $\mathbf{h}^k_{\mathcal{N}(u)} \leftarrow \text{AGGREGATE}_k(\{\mathbf{h}^{k-1}_{u'}, \forall u' \in \mathcal{N}_k(u)\})$;
    $\mathbf{h}^k_u \leftarrow \sigma\left(\mathbf{W}^k \cdot \text{CONCAT}(\mathbf{h}^{k-1}_u, \mathbf{h}^k_{\mathcal{N}(u)})\right)$;
    $\mathbf{h}^k_u \leftarrow \mathbf{h}^k_u / \|\mathbf{h}^k_u\|_2$;
  **end**
**end**

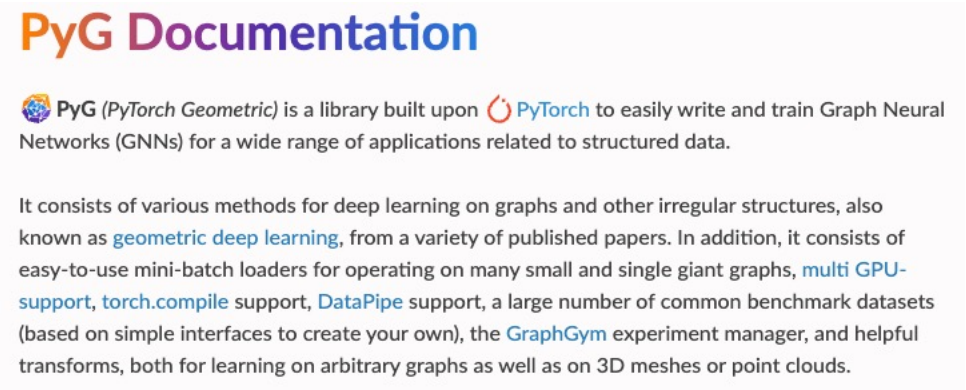



The <u>feed-forward process (message-passing)</u> is conceptually reversed compared to forward pass.

# Final note: Library for graph learning

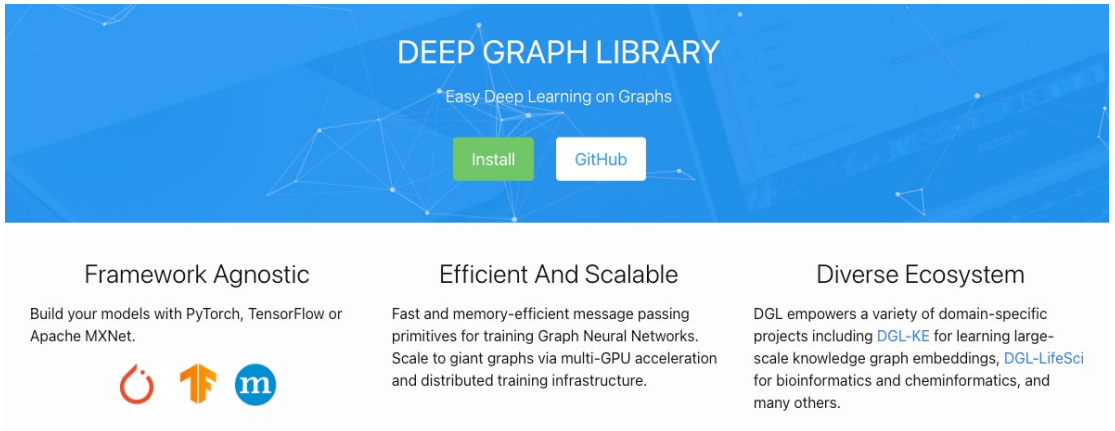
**Problem**: As we stack multiple layers, we introduce a **LOT** of neighboring nodes during message-passing.

**PyTorch Geometric** (link)




- Jure Leskovec (Standford/KumoAI/Snapchat)
- Faster library updates (is this a good thing?)
- (Seems like) A larger community

**Deep Graph Library** (link)



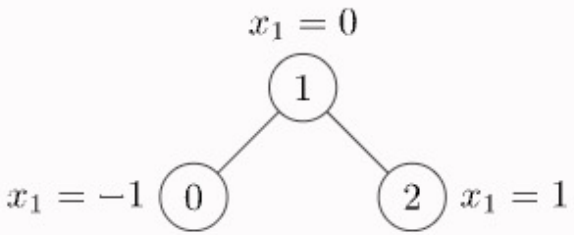

- Slower library updates (is this a bad thing?)
- Variable framework support

NetworkX
Network Analysis in Python

- Additonal library: NetworkX (link) – Library for graphs in general
  - Not a library for ML/DL
  - Often used in junction with PyG/DGL

# Final note: Library for graph learning

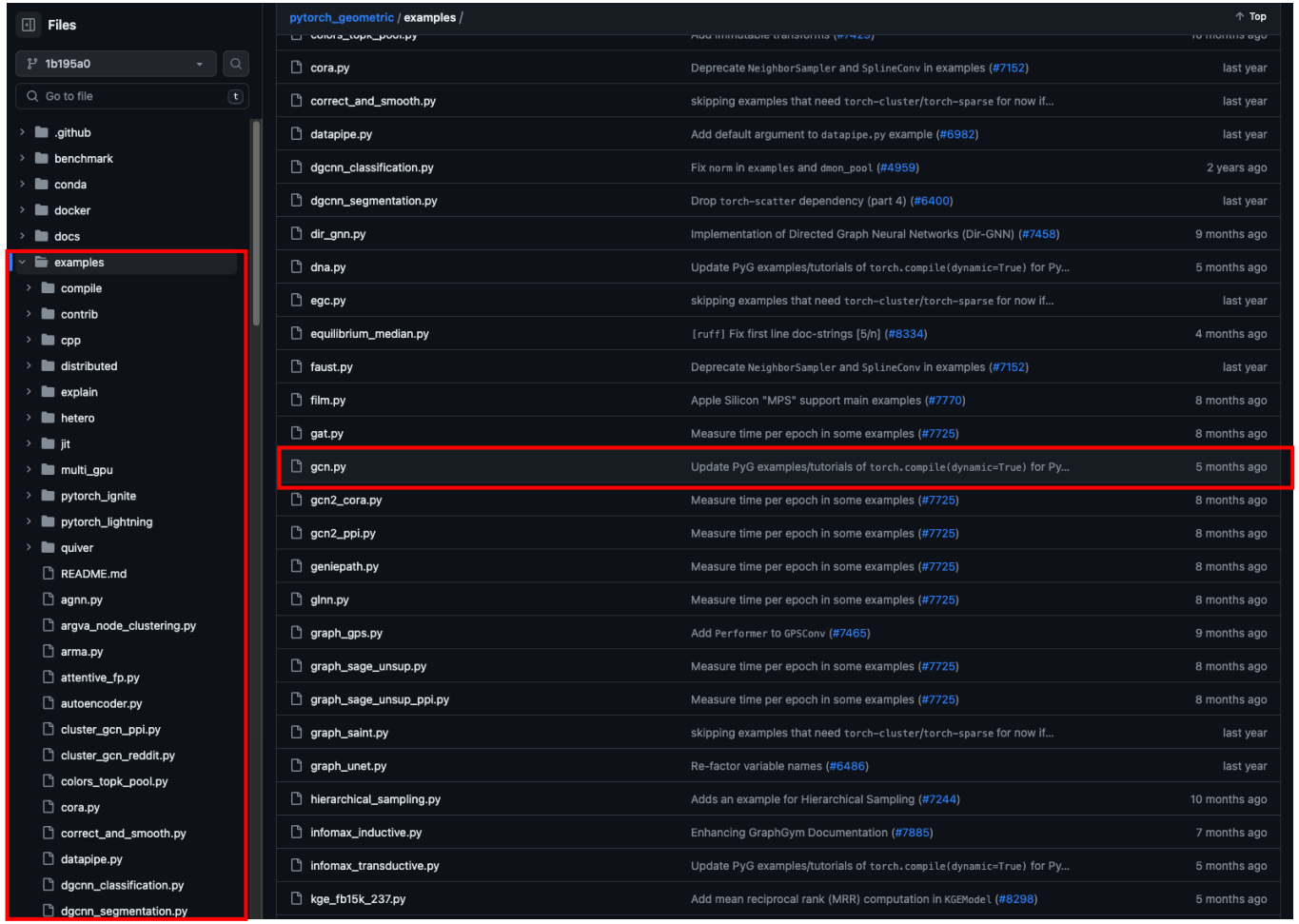
```python
import torch
from torch_geometric.data import Data

edge_index = torch.tensor([[0, 1, 1, 2],
                           [1, 0, 2, 1]], dtype=torch.long)
x = torch.tensor([[-1], [0], [1]], dtype=torch.float)

data = Data(x=x, edge_index=edge_index)
>>> Data(edge_index=[2, 4], x=[3, 1])
```




- You *at minimum* need to define data.edge_index
- Node features are usually represented as data.x
- Don't forget to include both directions for undirected graphs
- Most graph processing/manipulation tools are in torch_geometric.utils

# Final note: Library for graph learning

Go to the examples folder in the repo




If you want to know how to run GCN, go to the gcn.py file!

Includes…

- How to prep the data (with preprocessing, data splits etc.)
- How to define the model
- How to set up the training iteration
- How to measure performance

# Takeaways

1. Graphs are entities (nodes) that are **connected** (edges)
2. A lot of problems can be formulated as a graph learning problem
3. Graph neural networks = **Message-passing framework (Aggregate + Transformation)**

**Thank you!**

Please feel free to ask any questions :)

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