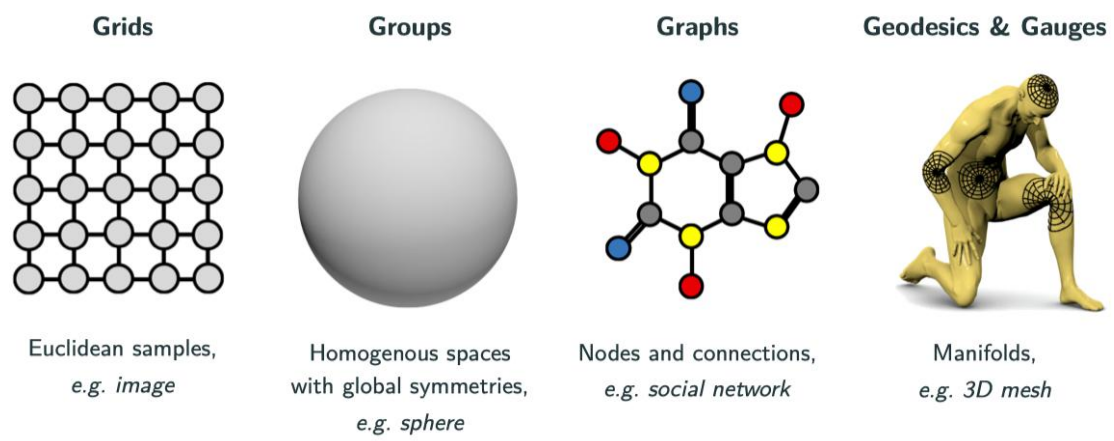


INTRODUCTION TO GRAPH REPRESENTATION LEARNING

Andreas Makris

LAI Reading Group



Images from NVIDIA, DeepMind,
Geometric Deep Learning Grids, Groups, Graphs, Geodesics, and Gauges

Resources

Presentation based on:

- Introduction to Graph Representation Learning
https://www.cs.mcgill.ca/~wlh/grl_book/files/GRL_Book.pdf
- Deep Graph-Based Learning Course
<https://github.com/basiralab/DGL/tree/main>

For people that like videos:

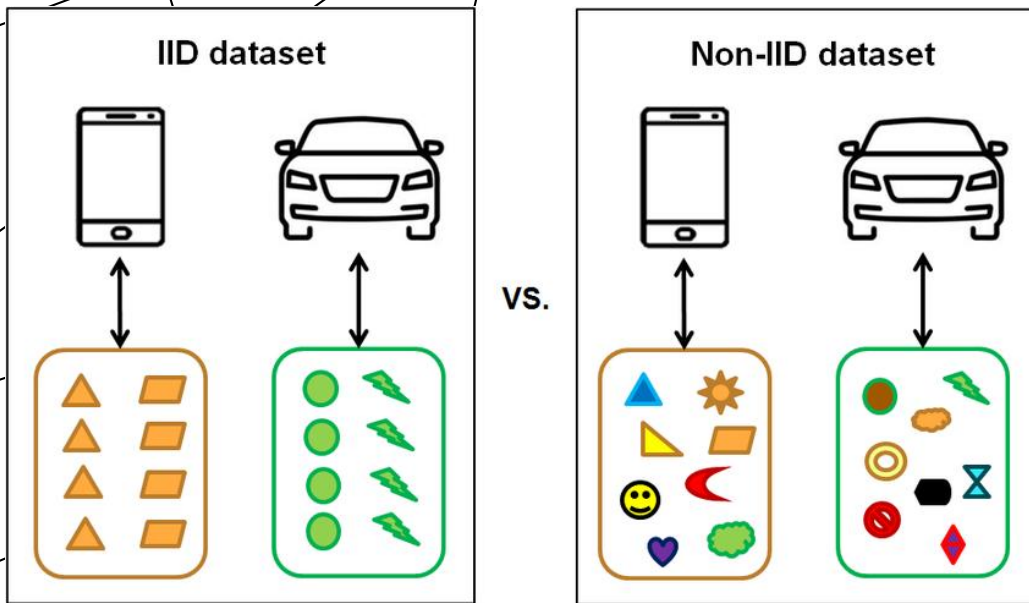
Stanford CS224W: Machine Learning with Graphs

<https://www.youtube.com/playlist?list=PLoROMvodv4rPLKxIpqhjhPg dQy7i mNkDn>

Deep Graph Learning

https://www.youtube.com/playlist?list=PLug43ldmRSo14Y_vt7S6vanPGh-JpHR7T

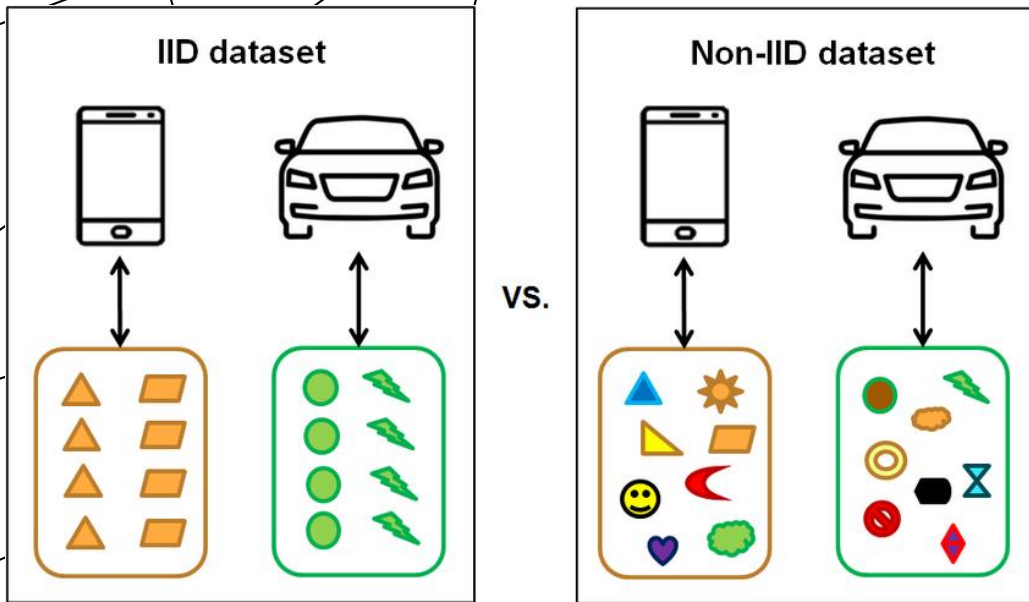
The Usual ML/DL Assumption



Our data is **independent** and **identically distributed**!

Image from Entropy to Mitigate Non-IID Data Problem on Federated Learning for the Edge Intelligence Environment

The Usual ML/DL Assumption

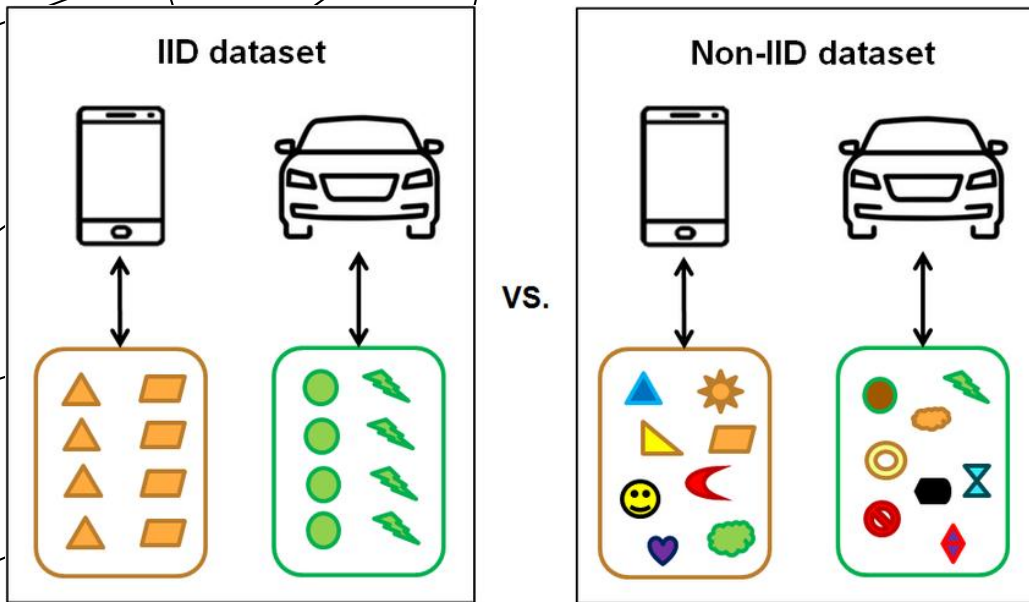


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What if it isn't?

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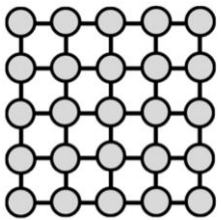
What if it isn't?

How can we use that to enhance our models?

Image from Entropy to Mitigate Non-IID Data Problem on Federated Learning for the Edge Intelligence Environment

Geometric Deep Learning

Grids



Euclidean samples,
e.g. image

Groups



Homogenous spaces
with global symmetries,
e.g. sphere

Graphs



Nodes and connections,
e.g. social network

Geodesics & Gauges



Manifolds,
e.g. 3D mesh

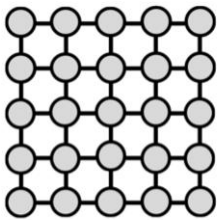
The structure of the data has additional information.

Inductive bias refers to the assumptions a learning algorithm makes to generalize beyond its training data.

Image from Geometric Deep Learning Grids, Groups, Graphs, Geodesics, and Gauges

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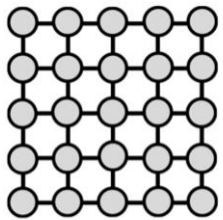
Geometric Deep Learning utilizes the structure of the data to improve our models.

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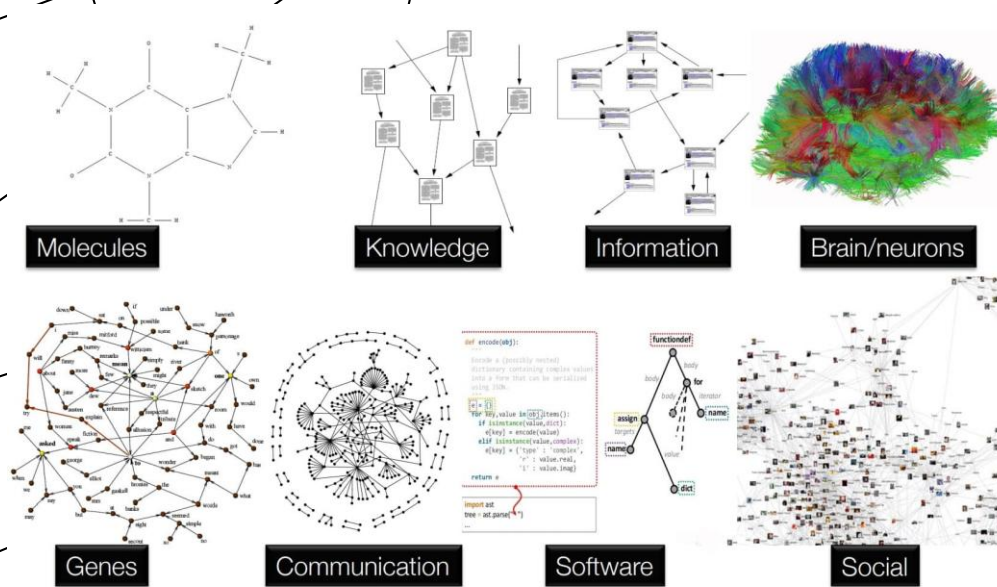
Geometric Deep Learning utilizes the structure of the data to improve our models.

We say we use **inductive bias** in our models.

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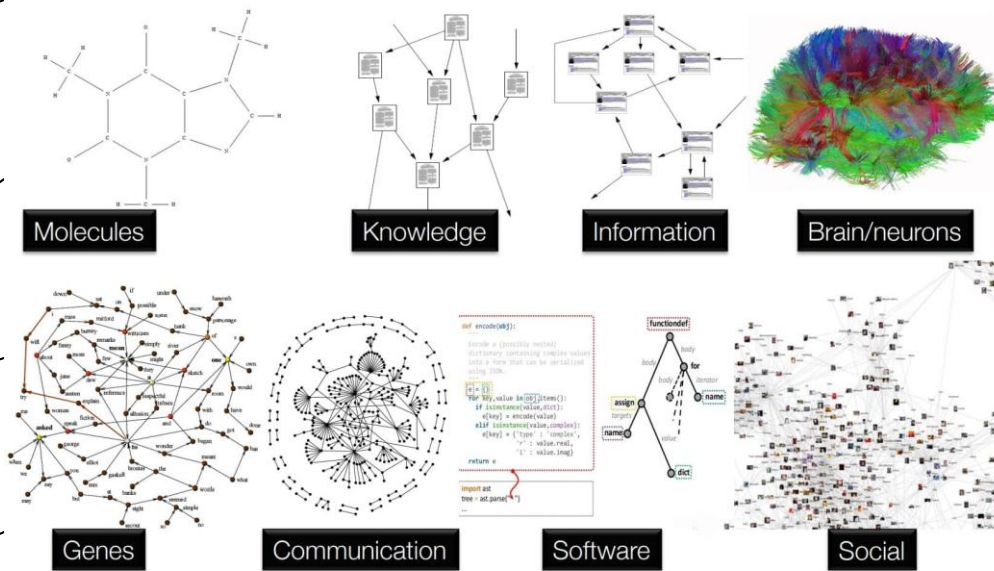
Graph Neural Networks



The most common and popular structure that we utilize in Deep Learning are graphs.

Image from <https://blogs.nvidia.com/blog/what-are-graph-neural-networks/>

Graph Neural Networks

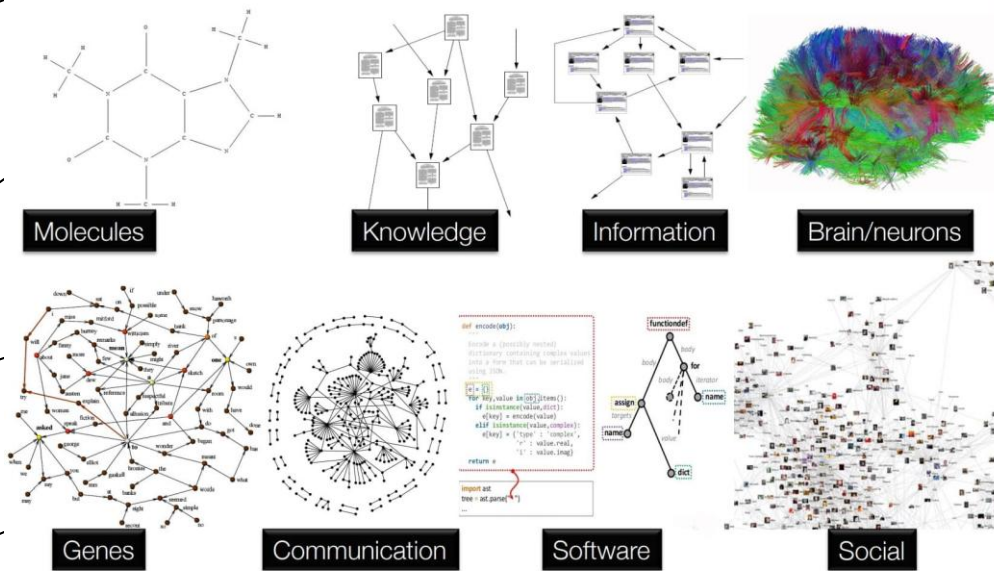


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Neural Network architectures/techniques that consider the graph-structure of the data.

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Graph Neural Networks



The most common and popular structure that we utilize in Deep Learning are graphs.

Neural Network architectures/techniques that consider the graph-structure of the data.

We will mainly focus on GNNs this term!

Image from <https://blogs.nvidia.com/blog/what-are-graph-neural-networks/>

Background for GNNs



Graph Theory

Deep Learning

Background for GNNs



The diagram features a central title 'Background for GNNs' at the top. Two arrows originate from this title: one points down and to the left towards a red-outlined box containing the text 'Graph Theory', and the other points down and to the right towards the text 'Deep Learning'. On the far left, there is a complex web of intersecting black lines that do not contain any text.

Graph Theory

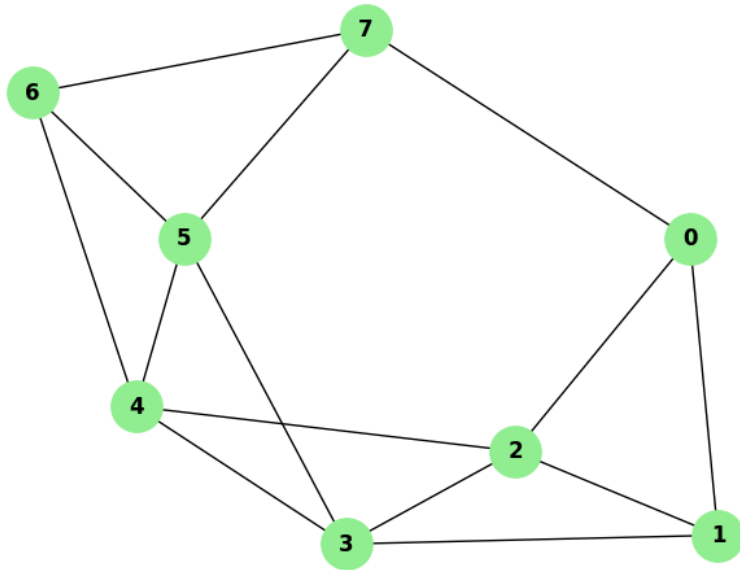
Deep Learning

We assume some ML/DL background.

This and next week we aim to gain some experience on Graph Theory and traditional ML for Graphs

What is a Graph?

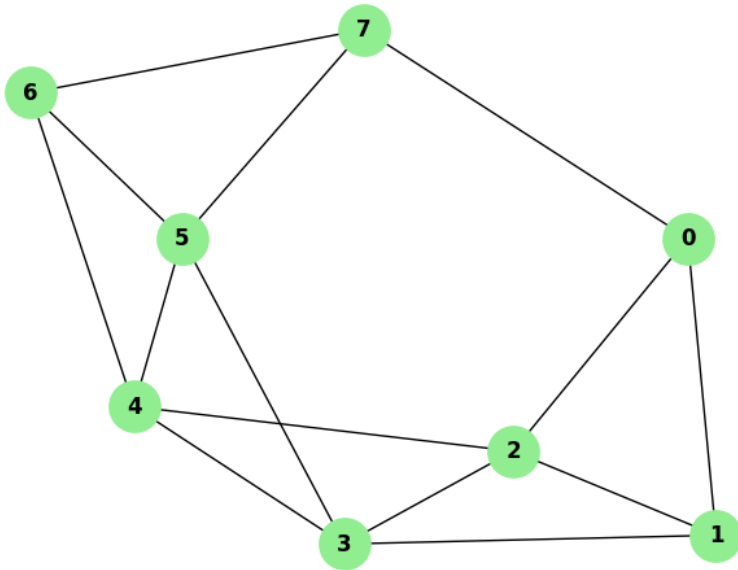
Graph



“A graph or a network is a collection of objects along with a set of interactions between pairs of these objects.” (GRL Book)

What is a Graph?

Graph

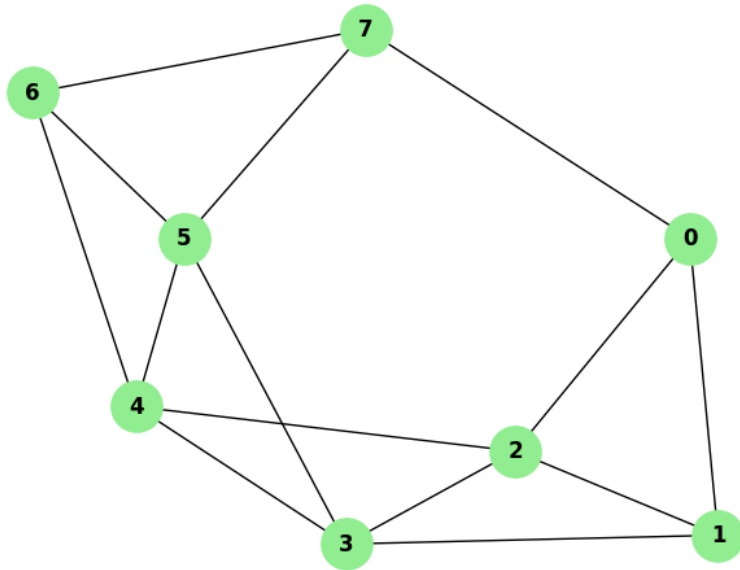


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“Formally, a graph $G = (V, E)$ is defined by a set of nodes V and a set of edges E between these nodes.” (GRL Book)

What is a Graph?

Graph



“A graph or a network is a collection of objects along with a set of interactions between pairs of these objects.” (GRL Book)

“Formally, a graph $G = (V, E)$ is defined by a set of nodes V and a set of edges E between these nodes.” (GRL Book)

For example, $V = \{0, 1, 2, 3, 4, 5, 6, 7\}$ and

$E = \{(0, 1), (0, 2), (0, 7), (1, 2), (1, 3), (2, 3), (2, 4), (3, 4), (3, 5), (4, 5), (4, 6), (5, 6), (5, 7), (6, 7)\}$

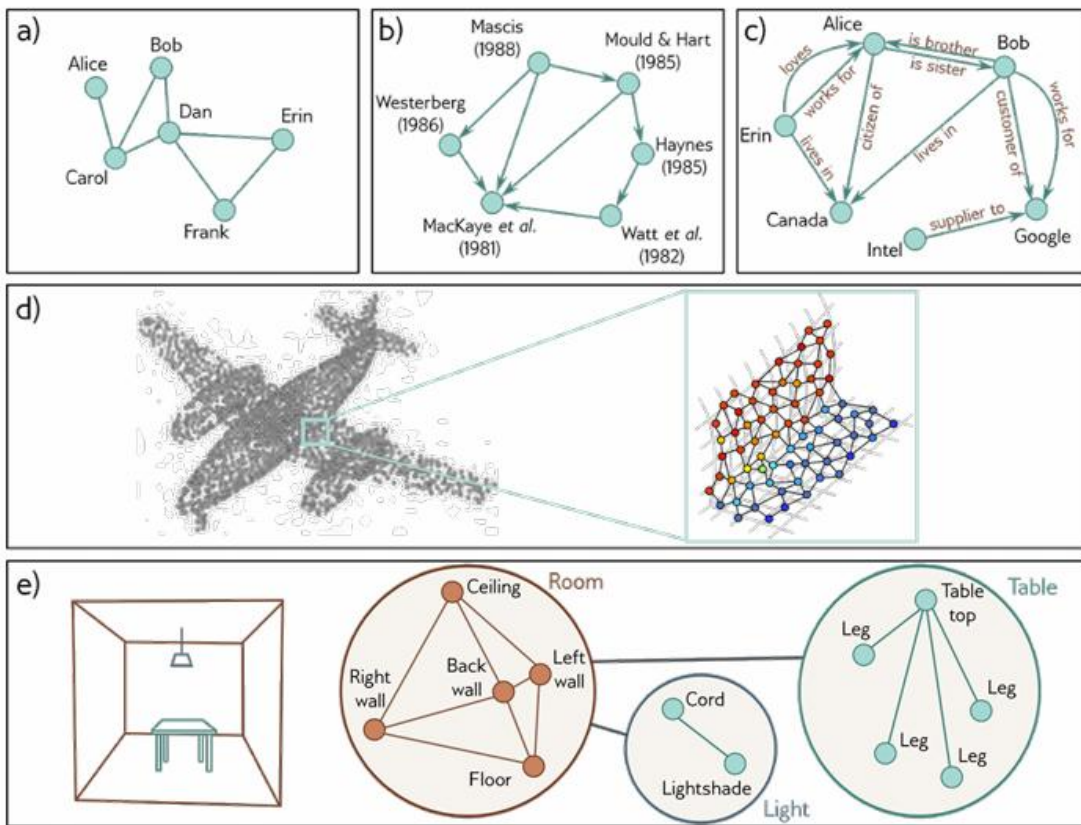


Figure 2 Types of graph. a) A social network is an undirected graph; the connections between people are symmetric. b) A citation network is a directed graph; one publication cites another, so the relationship is asymmetric. c) A knowledge graph is a directed heterogeneous multigraph. The nodes are heterogeneous in that they represent different object types (people, places, companies) and there may be multiple edges representing different relations between each node. d) A point set can be converted to a graph by forming edges between nearby points. Each node has an associated position in 3D space and this is termed a geometric graph (adapted from Hu et al. 2021). e) The scene on the left can be represented by a hierarchical graph. The topology of the room, table, and light are all represented by graphs and these graphs form nodes in a larger graph representing object adjacency (adapted from Fernández-Madrigal & González 2002).

Why do we care about Graphs?

Graphs are everywhere!

- Social Network Graph (nodes: individuals; edges: relationships or friendships)
- Computer Network Graph (nodes: computers, routers, or servers; edges: data connections or cables)
- Transportation Network Graph (nodes: cities or intersections; edges: roads, rail lines, or flight paths)
- Web Graph (nodes: webpages; edges: hyperlinks between pages)
- Molecule Structure Graph (nodes: atoms; edges: chemical bonds)
- Academic Papers Graph (nodes: authors; edges: whether they co-authored a paper)



Graph Learning Tasks

Node Level

Edge Level

Graph Level

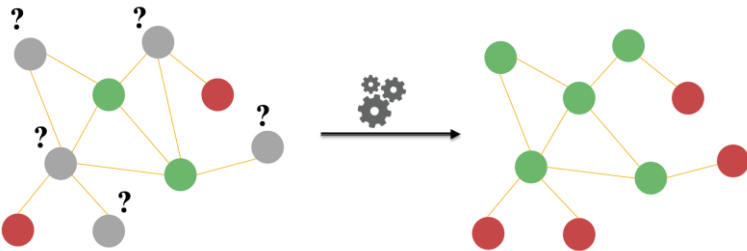
Graph Learning Tasks

Node Level

- Node classification/regression
e.g. price for each node
- Node clustering
- Representation learning (node embeddings)

Edge Level

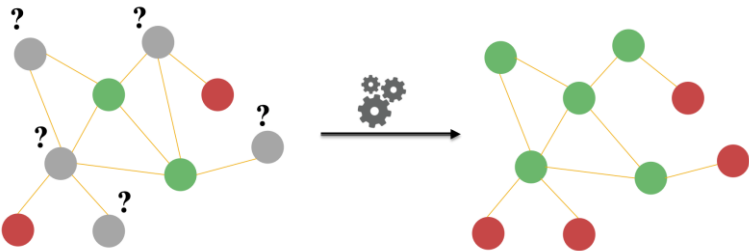
Graph Level



Graph Learning Tasks

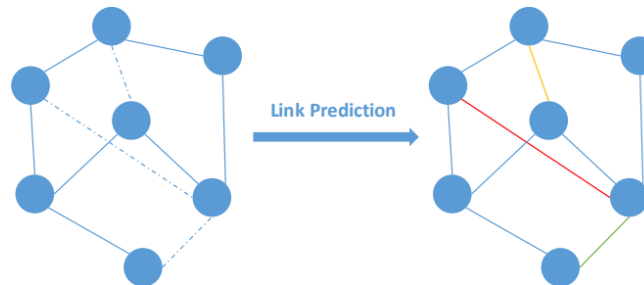
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Edge Level

- Edge classification/regression e.g. edges are transactions, fraud or not
- Link prediction e.g. recommend movies

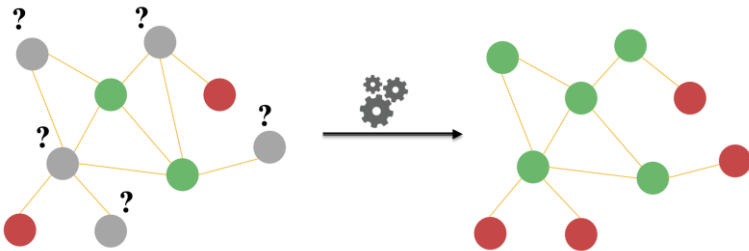


Graph Level

Graph Learning Tasks

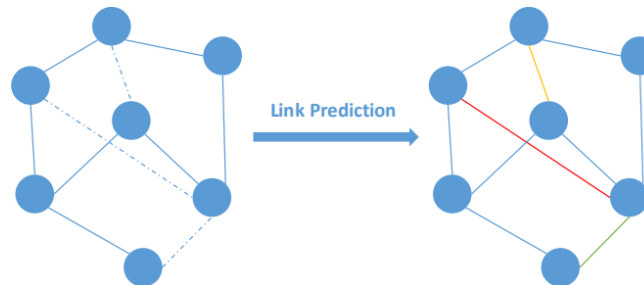
Node Level

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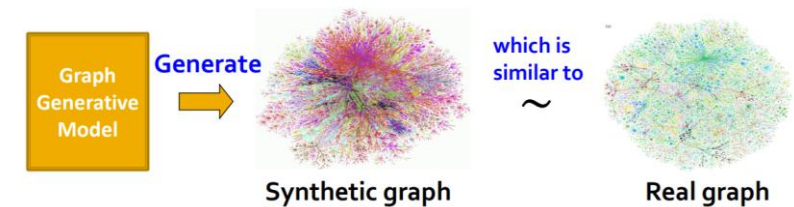
Edge Level

- Edge classification/regression e.g. edges are transactions, fraud or not
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Graph Level

- Graph classification/regression e.g. is the molecule toxic
- Graph clustering
- Graph generation e.g. create new molecules





How to use a Graph for ML?

How to use a Graph for ML?

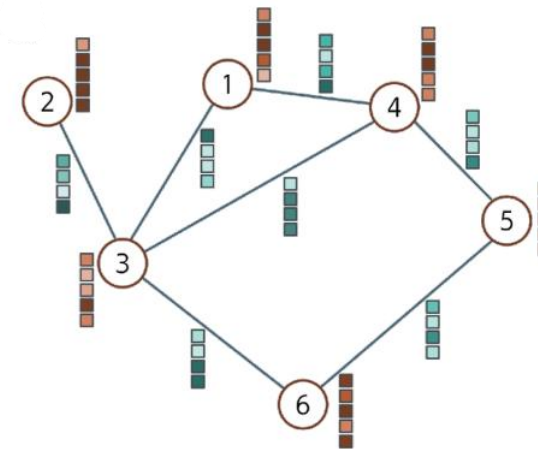
- Adjacency matrix **A** ($N \times N$)
- Node data **X** ($N \times D$)
- Edge data **E** ($N \times L$)
- Graph data (embedding for each graph)

N: number of nodes

D: node embedding dimension

L: edge embedding dimension

```
adj_matrix = np.array([
    #0  1  2  3  4  5  6  7
    [0, 1, 1, 0, 0, 0, 0, 1], # Node 0 connected to 1, 2, 7
    [1, 0, 1, 1, 0, 0, 0, 0], # Node 1 connected to 0, 2, 3
    [1, 1, 0, 1, 1, 0, 0, 0], # Node 2 connected to 0, 1, 3, 4
    [0, 1, 1, 0, 1, 1, 0, 0], # Node 3 connected to 1, 2, 4, 5
    [0, 0, 1, 1, 0, 1, 1, 0], # Node 4 connected to 2, 3, 5, 6
    [0, 0, 0, 1, 1, 0, 1, 1], # Node 5 connected to 3, 4, 6, 7
    [0, 0, 0, 0, 1, 1, 0, 1], # Node 6 connected to 4, 5, 7
    [1, 0, 0, 0, 0, 0, 1, 1]  # Node 7 connected to 0, 5, 6
])
```



How to use a Graph for ML?

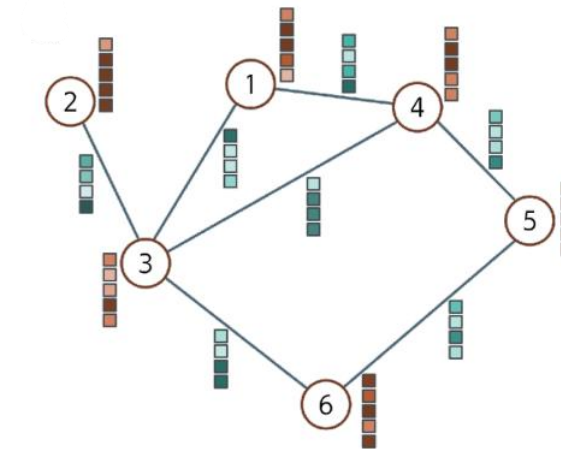
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adj_matrix = np.array([
    #0 1 2 3 4 5 6 7
    [0, 1, 1, 0, 0, 0, 0, 1], # Node 0 connected to 1, 2, 7
    [1, 0, 1, 1, 0, 0, 0, 0], # Node 1 connected to 0, 2, 3
    [1, 1, 0, 1, 1, 0, 0, 0], # Node 2 connected to 0, 1, 3, 4
    [0, 1, 1, 0, 1, 1, 0, 0], # Node 3 connected to 1, 2, 4, 5
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How do we get node/edge data?

How to use a Graph for ML?

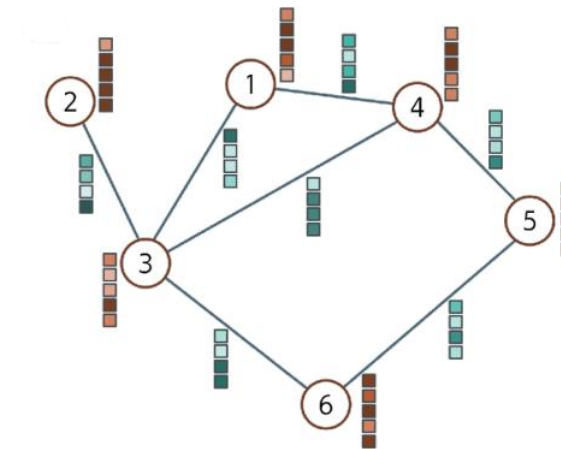
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N: number of nodes

D: node embedding dimension

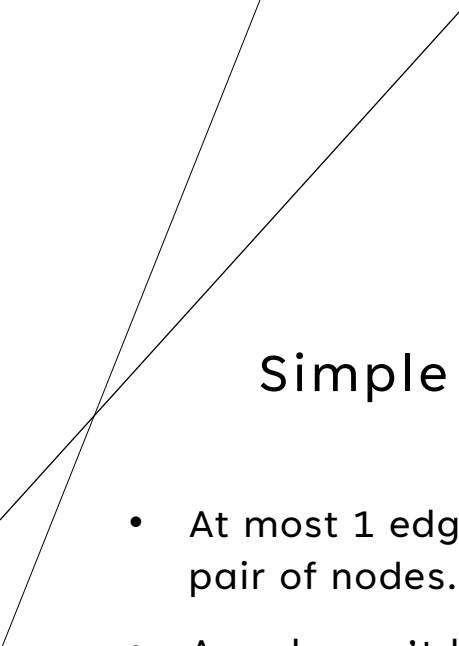
L: edge embedding dimension

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adj_matrix = np.array([
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])
```



How do we get node/edge data?

Before answering that, let's look at some types of graphs

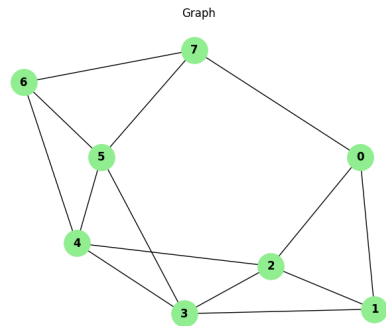


Simple

- At most 1 edge pair of nodes.
- A node can't

Simple Graphs

- At most 1 edge between each pair of nodes.
- A node can't have an edge with itself.
- Edges are undirected



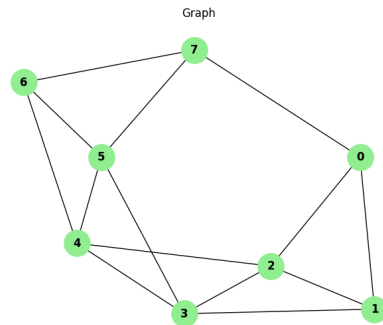
<https://graphicmaths.com/computer-science/graph-theory/adjacency-matrices/>

Wikipedia

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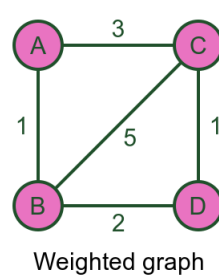


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Wikipedia

Weighted Graphs

- Weighted graphs have a weight associated with each edge. For example, distance to travel between cities.
- We usually use the weight matrix rather than the adjacency matrix.

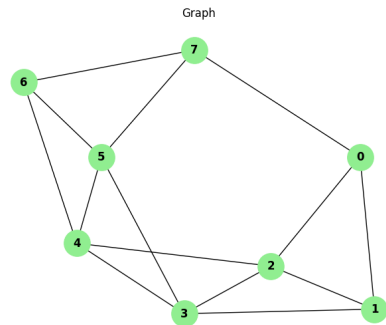


	A	B	C	D
A	0	1	3	0
B	1	0	5	2
C	3	5	0	1
D	0	2	1	0

Types of Graphs

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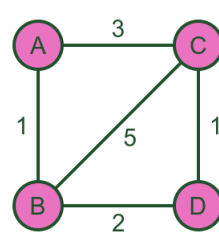


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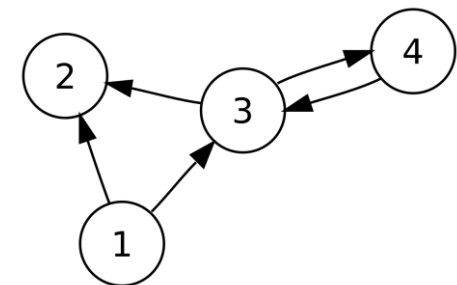


Weighted graph

	A	B	C	D
A	0	1	3	0
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C	3	5	0	1
D	0	2	1	0

Directed Graphs

- Edges have direction.



Multi-Relational Graphs

Graphs that have different types of edges. Then we get an adjacency tensor of shape $N \times \# \text{ of types of edges} \times N$. Example: relationship network, edges can be Facebook, Instagram, Twitter

[HMSG: Heterogeneous Graph Neural Network based on Metapath Subgraph Learning](#)

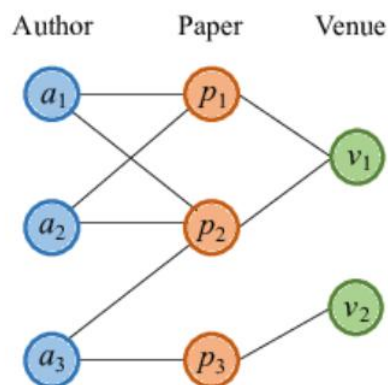
Learning embeddings for multiplex networks using triplet loss

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Heterogeneous Graphs

- We also have nodes of different types!
- Example: users and movies for recommender systems.



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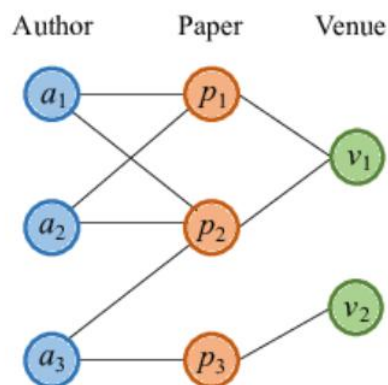
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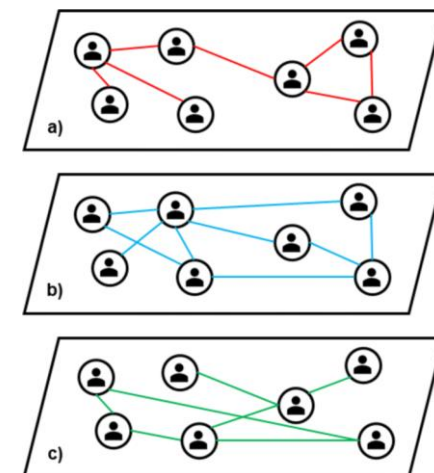


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Learning embeddings for multiplex networks using triplet loss

Multiplex Graphs

- The graph can be decomposed in a set of different layers.
- Each layer corresponds to a different type of edge.
- Example: Transportation network



ML for Graphs

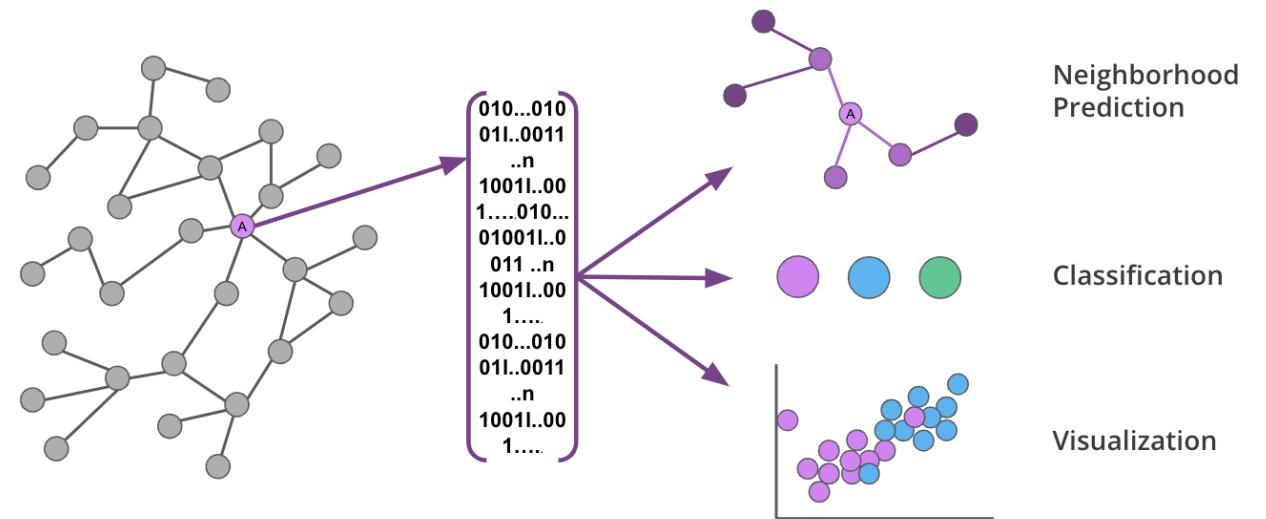
“ The challenge in these graph-level tasks, however, is how to define useful features that take into account the relational structure within each datapoint” – GRL Book

<https://neo4j.com/blog/machine-learning/announcing-graph-native-machine-learning-in-neo4j/>

ML for Graphs

“ The challenge in these graph-level tasks, however, is how to define useful features that take into account the relational structure within each datapoint” – GRL Book

1. Extract statistics for each node/edge/graph.
2. Use them as input to a standard ML model!

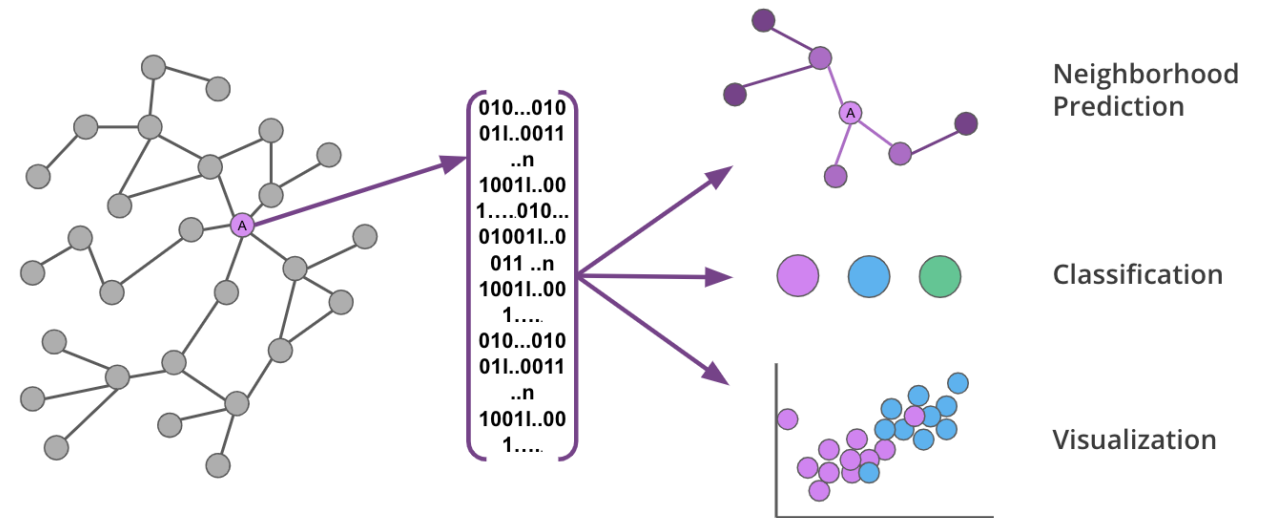


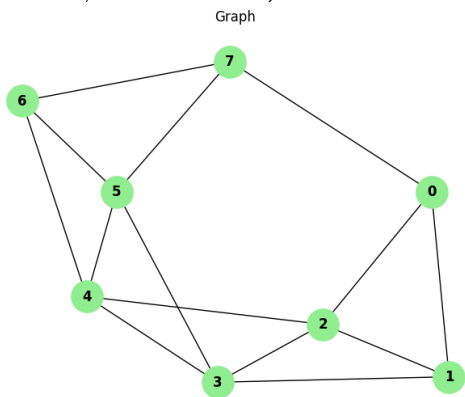
ML for Graphs

“ The challenge in these graph-level tasks, however, is how to define useful features that take into account the relational structure within each datapoint” – GRL Book

1. Extract statistics for each node/edge/graph.
2. Use them as input to a standard ML model!

What type of statistics can we extract





The Power of A

A^k is the matrix of the **number of paths of length k** between each pair of nodes!

Adjacency Matrix

0	1	1	0	0	0	0	0	1
1	0	1	1	0	0	0	0	0
1	1	0	1	1	0	0	0	0
0	1	1	0	1	1	0	0	0
0	0	1	1	0	1	1	1	0
0	0	0	1	1	0	1	1	1
0	0	0	0	1	1	0	1	1
0	0	0	0	1	1	0	1	1
1	0	0	0	0	1	1	0	0

A^{*2}

3	1	1	2	1	1	1	0
1	3	2	1	2	1	0	1
1	2	4	2	1	2	1	1
2	1	2	4	2	1	2	1
1	2	1	2	4	2	1	2
1	1	2	1	2	4	2	1
1	0	1	2	1	2	3	1
0	1	1	1	2	1	1	3

A^{*3}

2	6	7	4	5	4	2	5
6	4	7	8	4	4	4	2
7	7	6	9	9	5	4	4
4	8	9	6	9	9	4	5
5	4	9	9	6	9	8	4
4	4	5	9	9	6	7	7
2	4	4	4	8	7	4	6
5	2	4	5	4	7	6	2

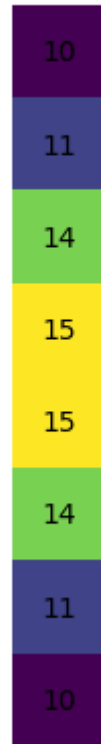
The Power of A

Each entry is the total number of k -step walks starting from the corresponding vertex in the graph

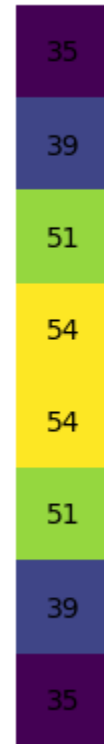
$A * e$



$A^2 * e$



$A^3 * e$



e is the unit vector

Node-level Statistics

- Node degree: number of edges a node is connected to. $d_u = \sum_{v \in V} \mathbf{A}[u, v].$

<https://networkx.org/documentation/stable/reference/algorithms/centrality.html>

Node-level Statistics

- Node degree: number of edges a node is connected to.
- Node centrality:
 - Considers how important a node's neighbours are.
 - There are many different centrality measures (e.g. eigenvector centrality, betweenness centrality).

$$d_u = \sum_{v \in V} \mathbf{A}[u, v].$$

<https://networkx.org/documentation/stable/reference/algorithms/centrality.html>

Node-level Statistics

- Node degree: number of edges a node is connected to. $d_u = \sum_{v \in V} \mathbf{A}[u, v].$
- Node centrality:
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 - There are many different centrality measures (e.g. eigenvector centrality, betweenness centrality).
 - Eigenvector centrality: “we define a node's eigenvector centrality via a recurrence relation in which the node's centrality is proportional to the average centrality of its neighbours” [GRL Book]. By Perron-Frobenius Theorem the vector of centrality values is given by the eigenvector corresponding to the largest eigenvalue of \mathbf{A} . Use power iteration to find that! **See GRL Book.**

$$e_u = \frac{1}{\lambda} \sum_{v \in V} \mathbf{A}[u, v] e_v \quad \forall u \in \mathcal{V} \quad \lambda \mathbf{e} = \mathbf{A} \mathbf{e}.$$

\mathbf{e} : vector of node centralities
 λ : constant

<https://networkx.org/documentation/stable/reference/algorithms/centrality.html>

Node-level Statistics

- Clustering coefficient:
 - Measures how tightly clustered a node's neighbourhood is.
 - Numerator: Number of edges between neighbours.
 - Denominator: Number of possible edges between the neighbours.

$$c_u = \frac{|(v_1, v_2) \in \mathcal{E} : v_1, v_2 \in \mathcal{N}(u)|}{\binom{d_u}{2}}$$

$$C_i = \frac{T_i}{\binom{d_i}{2}} = \frac{(A^3)_{ii}}{d_i(d_i - 1)}$$

<https://networkx.org/documentation/stable/reference/algorithms/centrality.html>

Graph-level Statistics

- Aggregate node-level statistics (e.g. histograms, means).

Edge Prediction

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- Count the number of neighbours that two nodes share or a normalised version of that!

$$\mathbf{S}[u, v] = |\mathcal{N}(u) \cap \mathcal{N}(v)| \quad \mathbf{S}_{\text{Sorenson}}[u, v] = \frac{2|\mathcal{N}(u) \cap \mathcal{N}(v)|}{d_u + d_v} \quad \mathbf{S}_{\text{Salton}}[u, v] = \frac{2|\mathcal{N}(u) \cap \mathcal{N}(v)|}{\sqrt{d_u d_v}}$$

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- We can also consider the importance of the common neighbors! (Resource Allocation, Adamic-Adar Index)

$$\mathbf{S}_{\text{RA}}[v_1, v_2] = \sum_{u \in \mathcal{N}(v_1) \cap \mathcal{N}(v_2)} \frac{1}{d_u} \quad \mathbf{S}_{\text{AA}}[v_1, v_2] = \sum_{u \in \mathcal{N}(v_1) \cap \mathcal{N}(v_2)} \frac{1}{\log(d_u)}$$

Edge Prediction

- There also exist global overlap measures like the Katz index that count the number of paths of all lengths between a pair of nodes.

$$\mathbf{S}_{\text{Katz}}[u, v] = \sum_{i=1}^{\infty} \beta^i \mathbf{A}^i[u, v]$$

β is a hyperparameter controlling how much weight is given to short versus long paths

- A theorem allows us to calculate that.

$$\mathbf{S}_{\text{Katz}} = (\mathbf{I} - \beta \mathbf{A})^{-1} - \mathbf{I}$$

The Problem with Traditional Approaches

- “The approaches discussed are limited due to the fact that **they require careful, hand-engineered statistics** and measures. These hand-engineered features are **inflexible**—i.e., they cannot adapt through a learning process—and designing these features can be a **time-consuming and expensive** process.” GRL Book

Degree Normalisation

- If we use the standard adjacency matrix for ML/DL the nodes with high degrees will “overwhelm” the model. We need to do some type of normalization!

$$\tilde{A} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

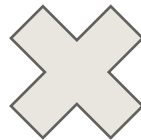
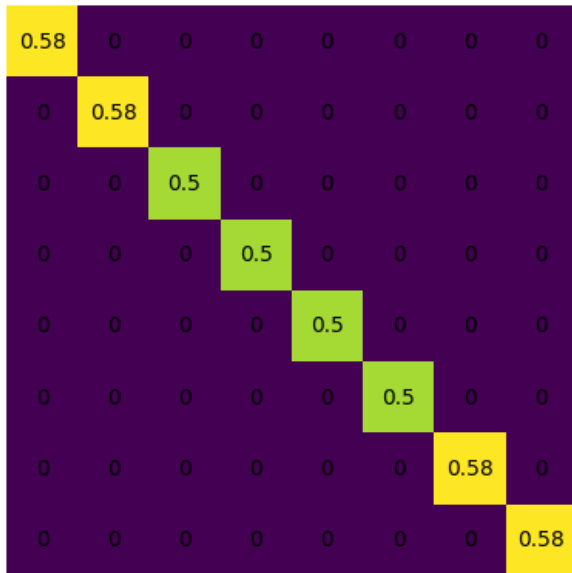
- What does the above calculation do exactly? Let’s look at an example.

Degree Normalisation

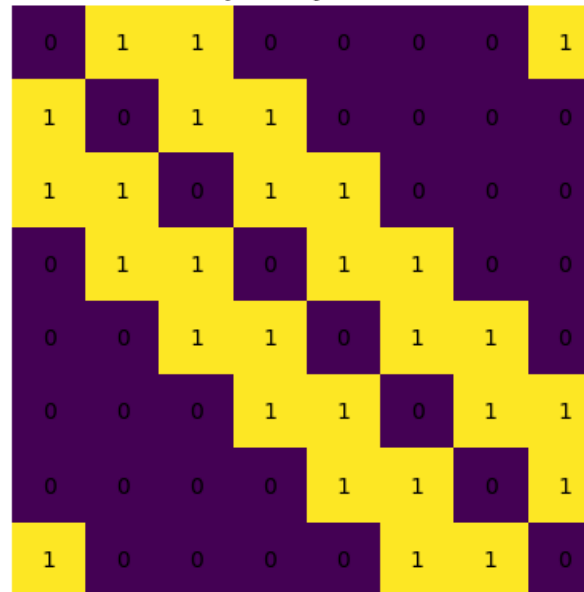
$$D^{-\frac{1}{2}} A$$

- The **left** multiplication multiplies each **row** by the number in the diagonal. Here, we divide each edge by the (sqrt) degree of the **left** node.

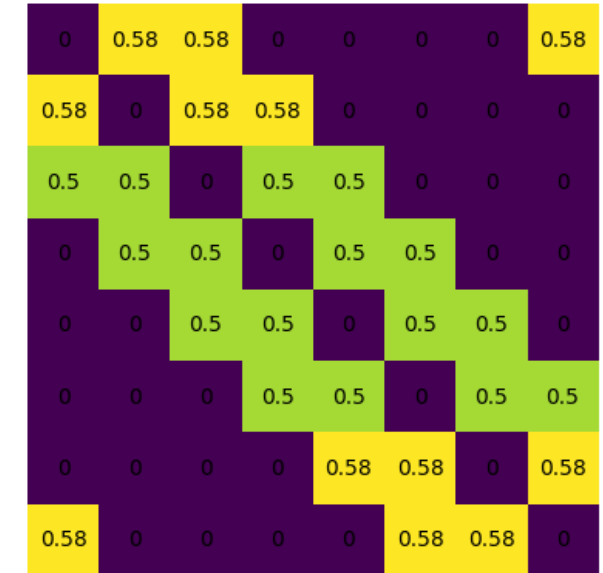
$D^{-1/2}$



Adjacency Matrix



$D^{-1/2}A$



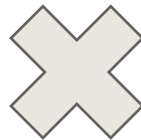
Degree Normalisation

$$AD^{-\frac{1}{2}}$$

- The **right** multiplication multiplies each **column** by the number in the diagonal. Here, we divide each edge by the (sqrt) degree of the **right** node.

Adjacency Matrix

0	1	1	0	0	0	0	0	1
1	0	1	1	0	0	0	0	0
1	1	0	1	1	0	0	0	0
0	1	1	0	1	1	0	0	0
0	0	1	1	0	1	1	0	0
0	0	0	1	1	0	1	1	0
0	0	0	0	1	1	0	1	1
0	0	0	0	1	1	0	0	1
1	0	0	0	0	1	1	0	0



$D^{-1/2}$

0.58	0	0	0	0	0	0	0	0
0	0.58	0	0	0	0	0	0	0
0	0	0.5	0	0	0	0	0	0
0	0	0	0.5	0	0	0	0	0
0	0	0	0	0.5	0	0	0	0
0	0	0	0	0	0.5	0	0	0
0	0	0	0	0	0	0.5	0	0
0	0	0	0	0	0	0	0.58	0
0	0	0	0	0	0	0	0	0.58



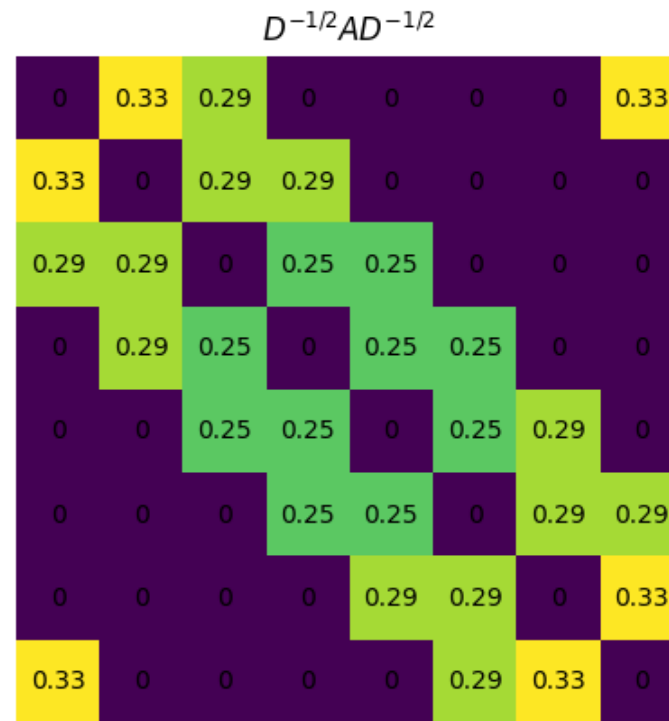
$AD^{-1/2}$

0	0.58	0.5	0	0	0	0	0	0.58
0.58	0	0.5	0.5	0	0	0	0	0
0.58	0.58	0	0.5	0.5	0	0	0	0
0	0.58	0.5	0	0.5	0.5	0	0	0
0	0	0.5	0.5	0	0.5	0.58	0	0
0	0	0	0.5	0.5	0	0.58	0.58	0
0	0	0	0	0.5	0.5	0	0.58	0.58
0	0	0	0	0	0.5	0.5	0	0.58
0.58	0	0	0	0	0	0.5	0.58	0

Degree Normalisation

- So, this is equivalent to

$$\frac{A_{ij}}{\sqrt{d_i} \sqrt{d_j}}$$

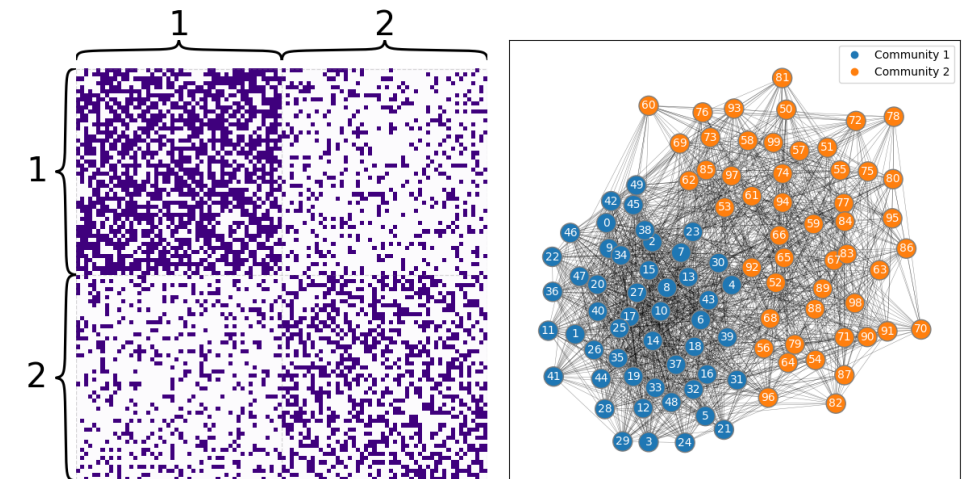


Sneak Peak for Next Week 🧐

- What about node clustering?
- What about learning embeddings for each node?
- Graph Laplacians and Spectral Methods
- Unnormalised Laplacian Matrix: $\mathbf{L} = \mathbf{D} - \mathbf{A}$

\mathbf{D} is the degree matrix (diagonal entries, diagonal matrix)

A, a sample from an $SBM_n(z, B)$ Simulation



<https://docs.neurodata.io/graph-stats-book/representations/ch6/spectral-embedding.html>

Key Takeaways

- We can include **inductive biases** to improve our models.
- Graphs are everywhere!
- The **adjacency matrix** of a matrix has many cool properties.
- For traditional ML, graph tasks require hand-crafted features which are **time-consuming** and **inflexible**.



THANK YOU
QUESTIONS?