Machine Learning with Graphs

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Why Graphs?

- Graphs are a universal language for understanding relationships and interactions.
- What data can we model as graphs?

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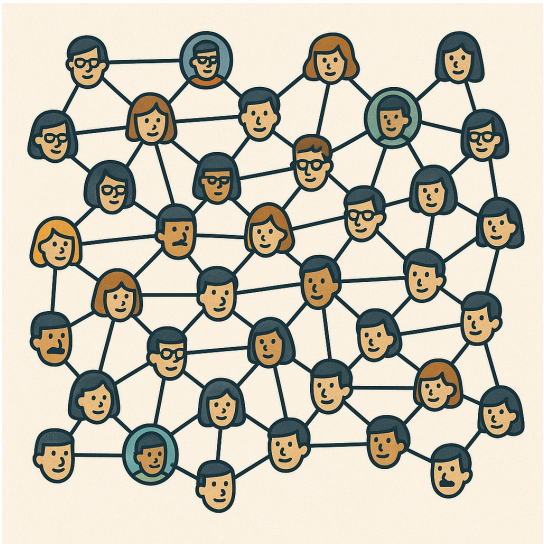
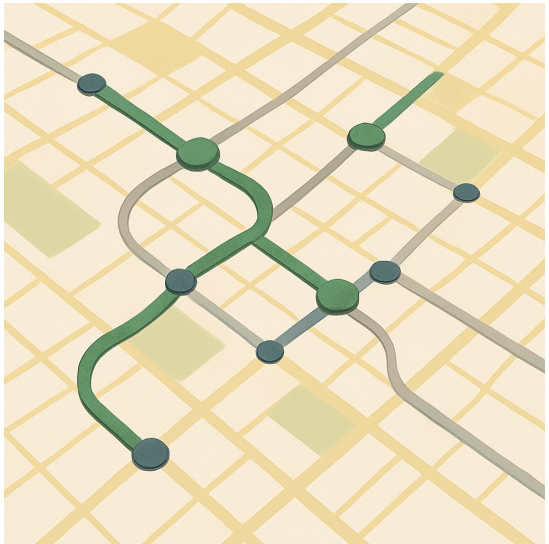


Social Networks

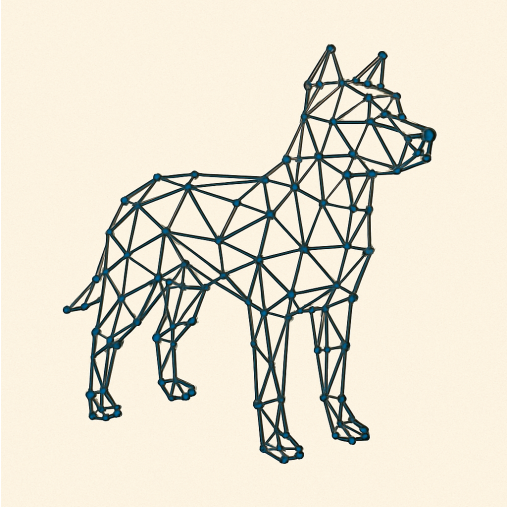
Computer Networks



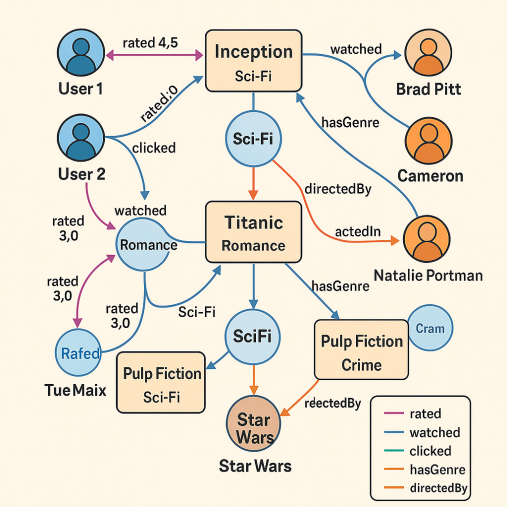
Road Networks

Why Graphs?

Citation Networks

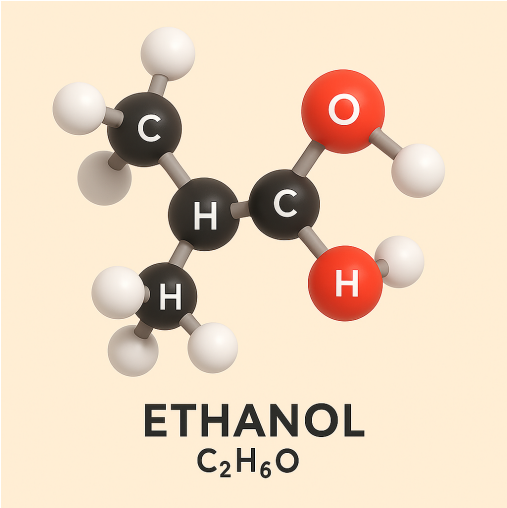


3D Meshes

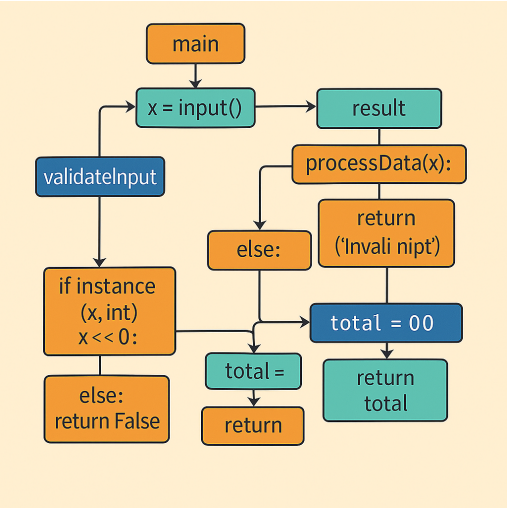


Recommender Graphs

Brain Connectomes



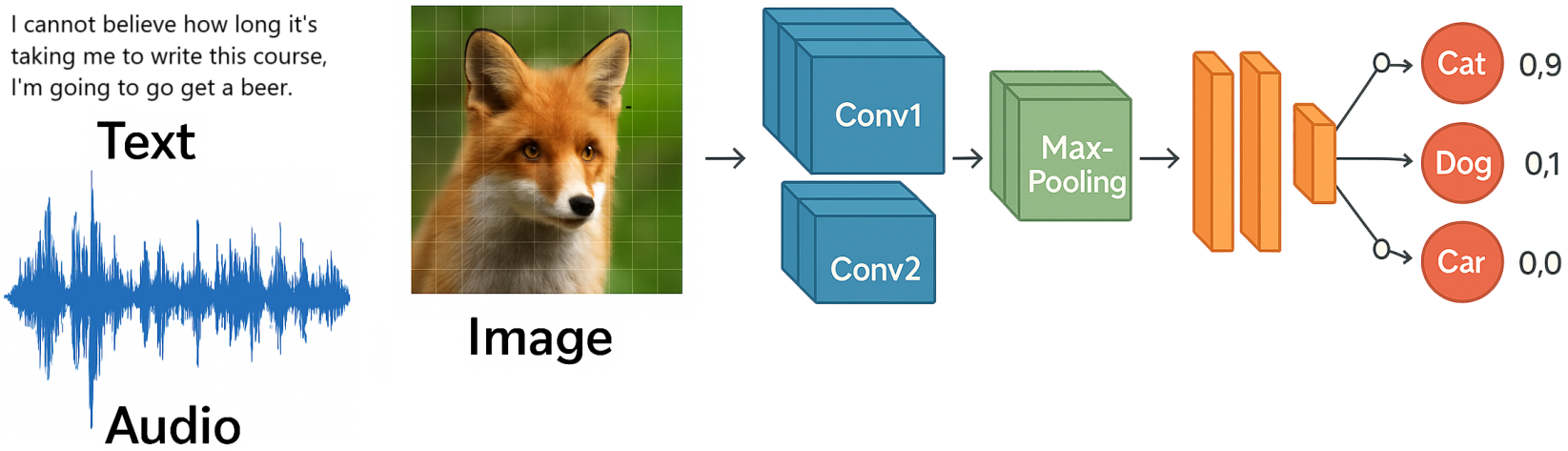
Molecular Graphs



Program Code Graphs

Why Graphs? Limitations of Traditional Deep Learning

- **Modern deep learning models** — such as **CNNs**, **RNNs**, and **Transformers** — are designed to operate on data organized as **grids** (e.g., images) or **sequences** (e.g., text, time series).
- These formats are:
  - Well understood
  - Supported by **highly optimized architectures**
  - Ideal for domains like computer vision, NLP, and time-series prediction



But There's a Gap...

Why Traditional Models Fall Short

- Many real-world problems involve **complex relationships** between entities:
  - Social connections
  - Biological interactions
  - Recommender systems
  - Scientific structures (e.g., molecules)
- These dependencies **don't fit neatly into a grid or sequence.**

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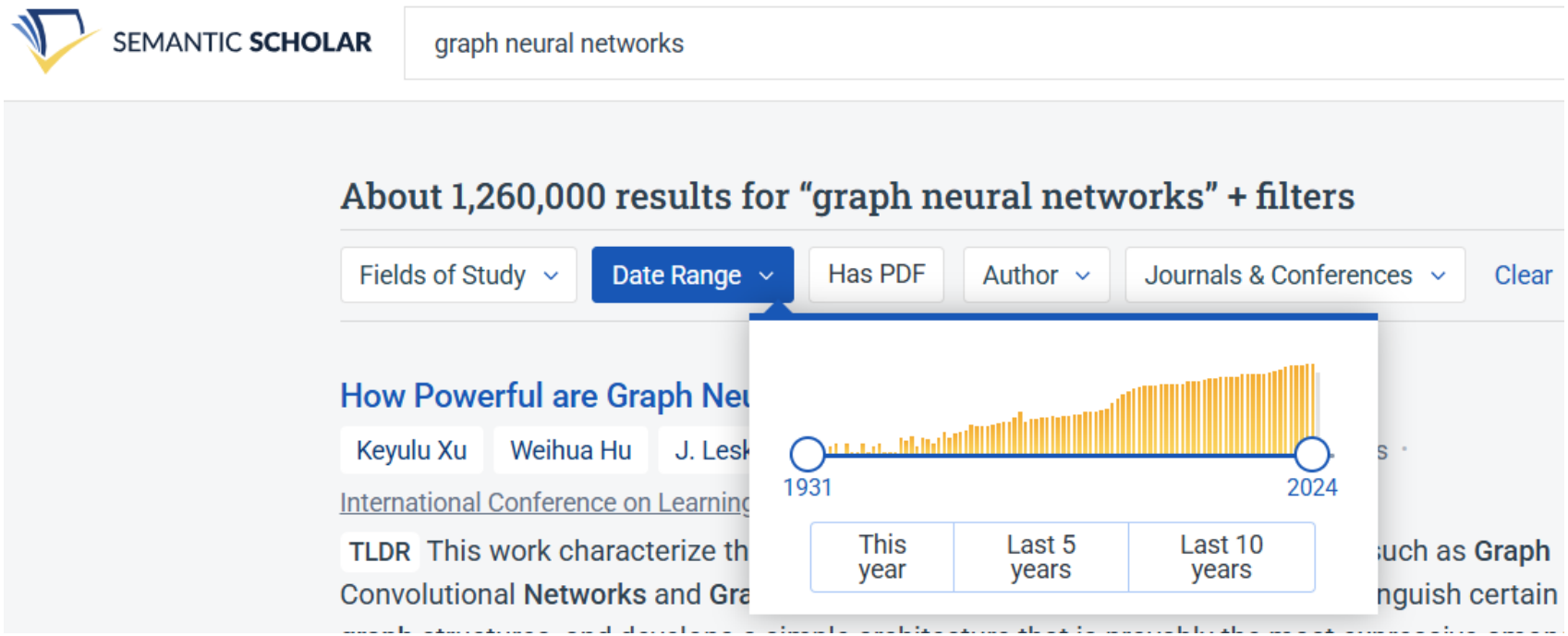
Graphs Fill This Gap

Graphs enable flexible, relational representations
*where structure is **irregular**, **sparse**, and **non-Euclidean** —*
and traditional deep learning models struggle.

The Rise of Graph Neural Networks

- Research on Graph Neural Networks (GNNs) has grown dramatically over the past decade.
- The figure below shows the increasing number of papers published each year with "Graph Neural Networks" in their title.



Why GNNs Are More Than Just a Trend

- GNNs combine the structure of graphs with the predictive power of deep learning.
- They can learn sophisticated node and edge representations (embeddings).
- Real-world systems actively use them for tasks requiring relational reasoning.
- Their key strength: capturing both node attributes and relationships between entities.

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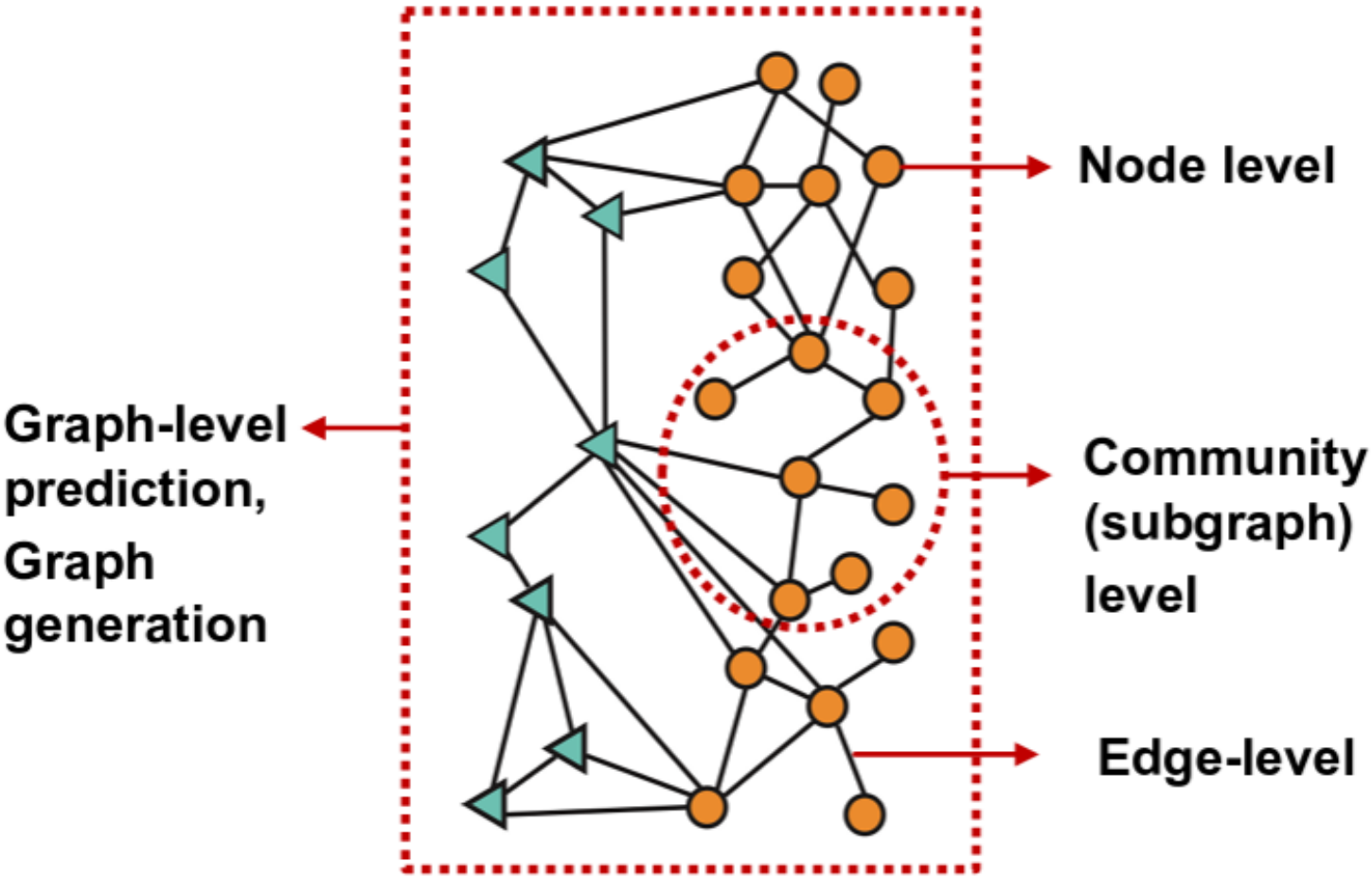
Is My Problem a Graph Problem?

If your data has natural **connections or interdependencies** between entities — users, products, merchants, documents — it may benefit from a graph-based approach.

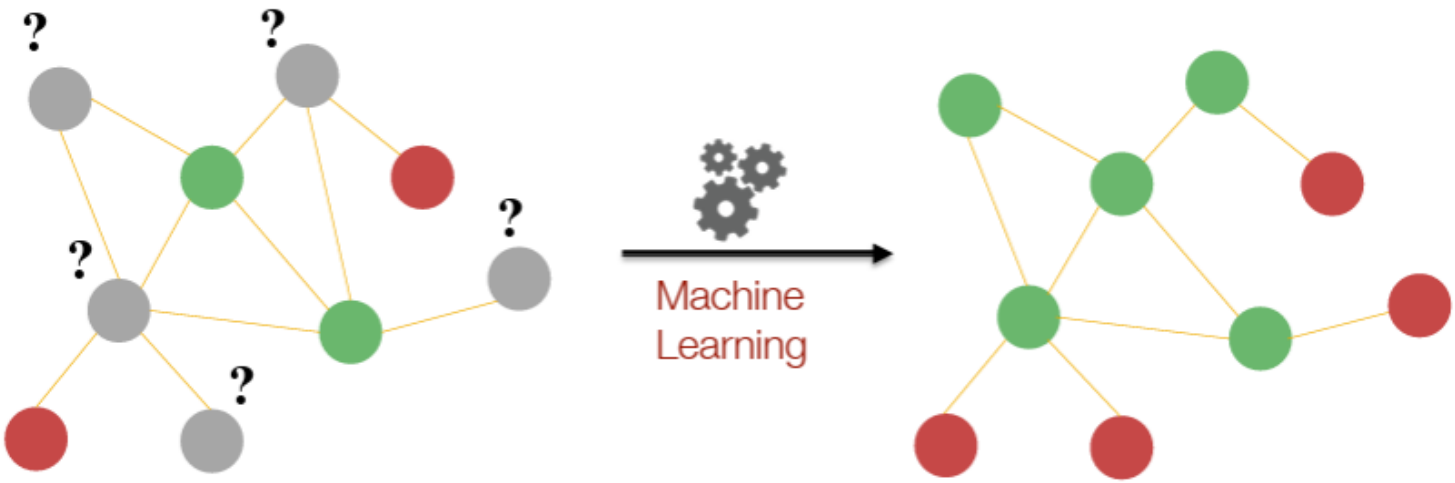
Types of Tasks



Node-Level Tasks

Goal

Predict a label, category, or attribute for each individual node within a graph.



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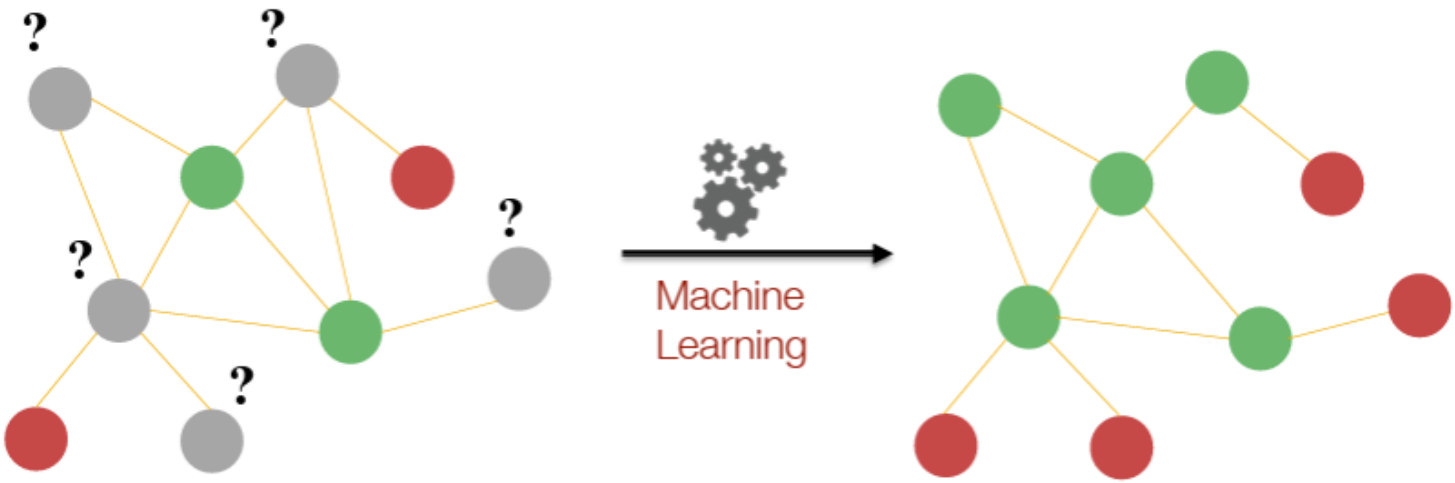


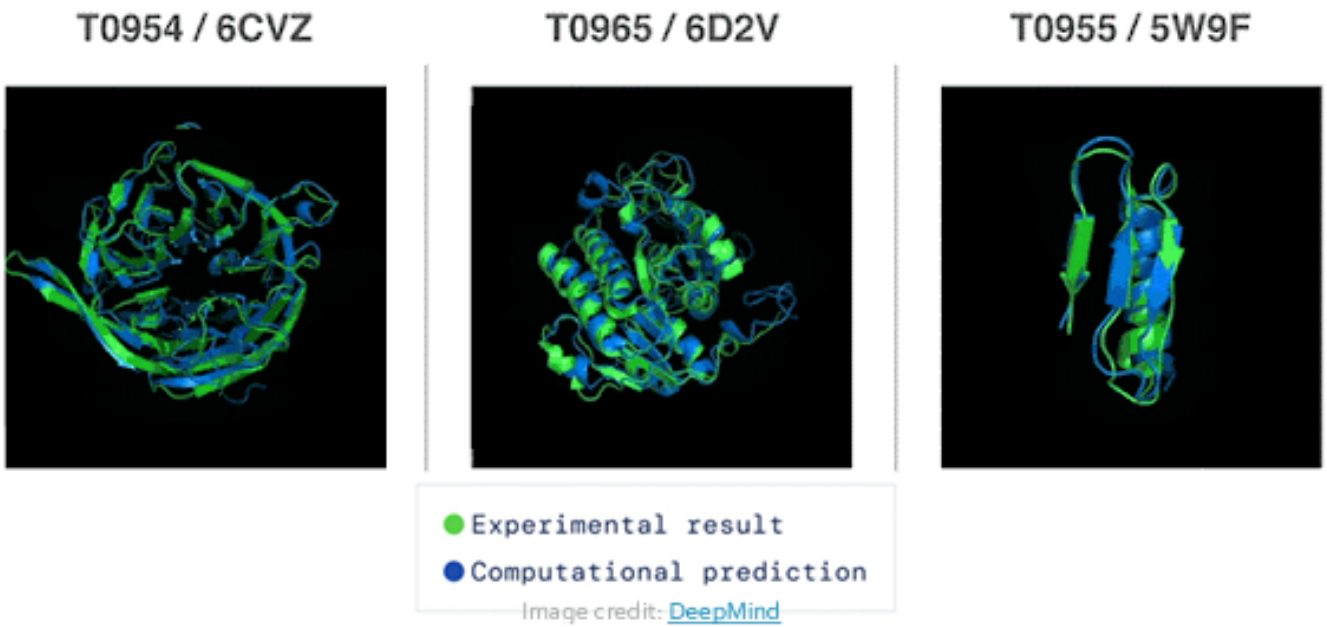
Common tasks include:

- **Node classification** (e.g., user type, document topic)
- **Node regression** (e.g., ranking score, age prediction)

Example: Node-Level Regression for Protein Folding

Breakthrough: Predicting Protein Structures with GNNs

- Recent advances in deep learning, notably by DeepMind's **AlphaFold**, have revolutionized the protein folding problem.
- Proteins can be modeled as **graphs**, where:
  - **Nodes:** Amino acids (residues) in the protein sequence
  - **Edges:** Spatial proximity or learned interaction between residues
  - **Task:** For each node, **predict its 3D coordinates** (x, y, z)



Example: Node-Level Regression for Protein Folding

Why Graph Neural Networks?

- Proteins are naturally irregular, flexible, and structured — ideal for graphs
- Their folded structure depends on long-range, non-local interactions — not just sequence order.
- GNNs enable message passing between residues to learn spatial dependencies
- Enables accurate modeling of physical constraints and folding behavior

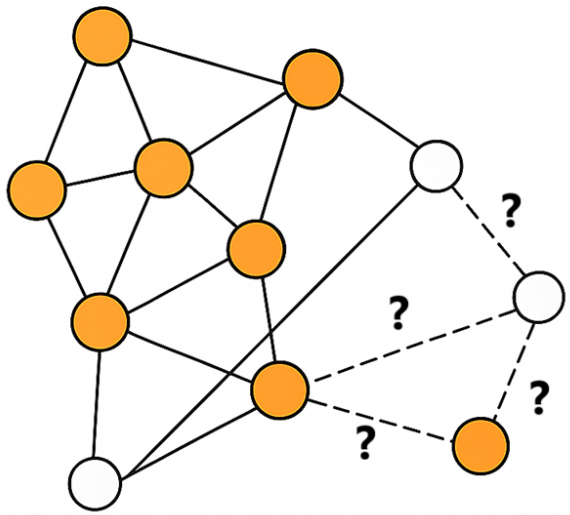
Why It Matters

AlphaFold achieved near-experimental accuracy in predicting protein 3D structures, solving a 50-year grand challenge in biology — enabled in part by graph-based learning.

Edge-Level Tasks

Goal

- Predict whether an **edge exists** between two nodes — even if it is currently missing or unknown.
- At test time: Given a set of node pairs with **no existing edge**, assign a score to each pair and **rank** them.
- The top-K ranked pairs are predicted as new or likely edges.
- It is essentially a **binary classification / scoring task** over node pairs.



Example: Edge-Level Prediction for Recommender Systems

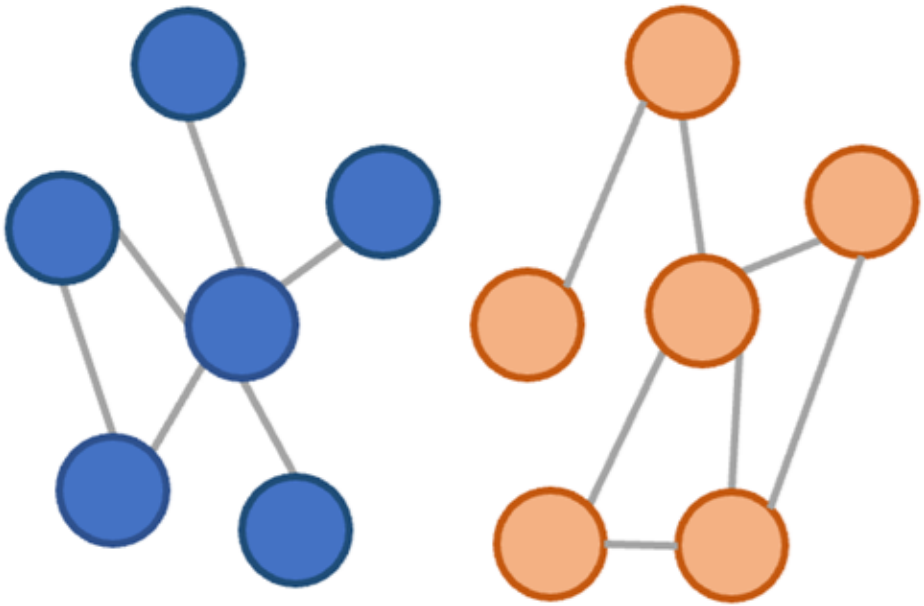
Problem Setting

- Model user-item interactions as a bipartite graph:
  - **Nodes:** Users and items (e.g., movies, books, products)
  - **Edges:** Observed interactions (e.g., rating, click, purchase)
- Goal: **Predict new edges** between users and items they haven't interacted with yet.
- This is a classic **link prediction** task on a bipartite graph.

Graph-Level Tasks

What Are Graph-Level Tasks?

- The goal is to predict a label, property, or output for an entire graph — not individual nodes or edges.
- The model learns a **global representation (embedding)** of the entire graph structure and features.

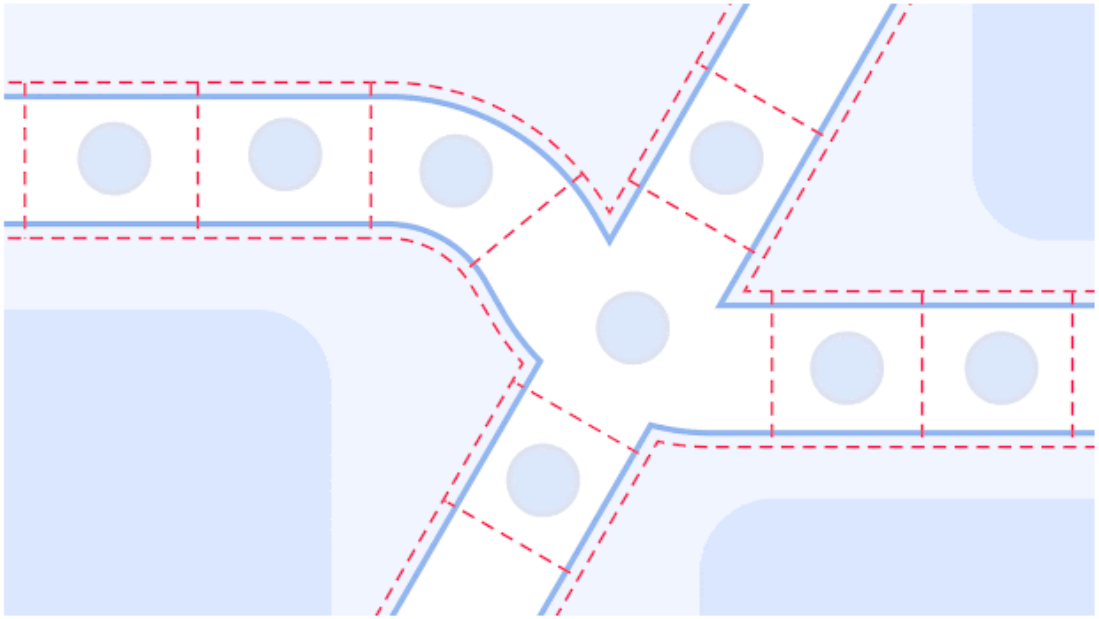


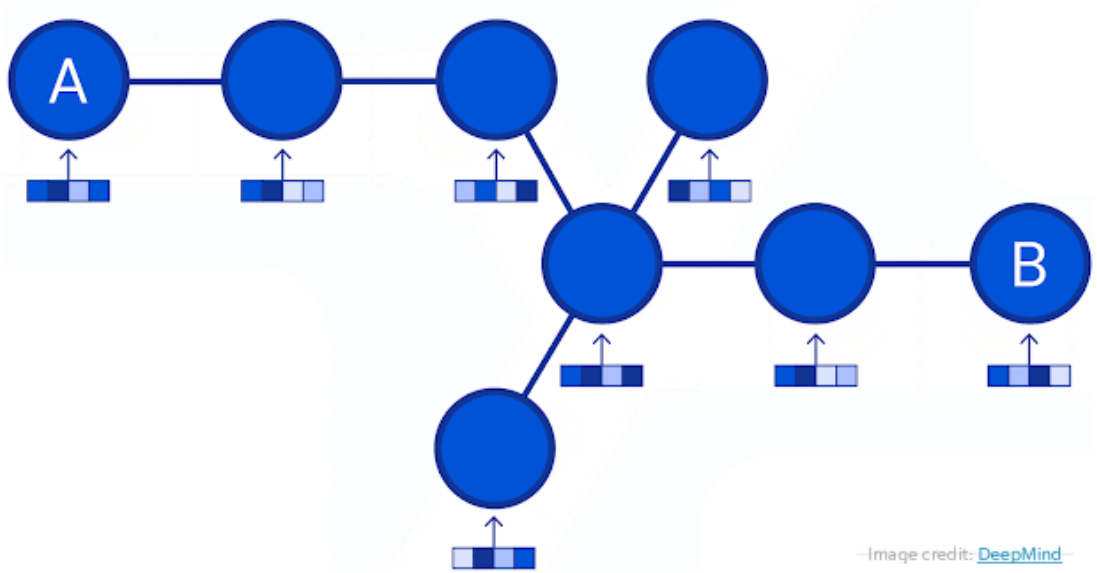
Example: ETA Predictions in Google Maps

Problem Setting

- Road Network as a Graph
  - **Nodes:** Represent road segments or intersections.
  - **Edges:** Connectivity between road segments / intersections (roads).
- Task: Predict the **Time of Arrival (ETA)** at the destination given the starting point.
- Use **real-time traffic data** (traffic congestion, accidents) to adjust the travel time along each road segment.

Example: ETA Predictions in Google Maps





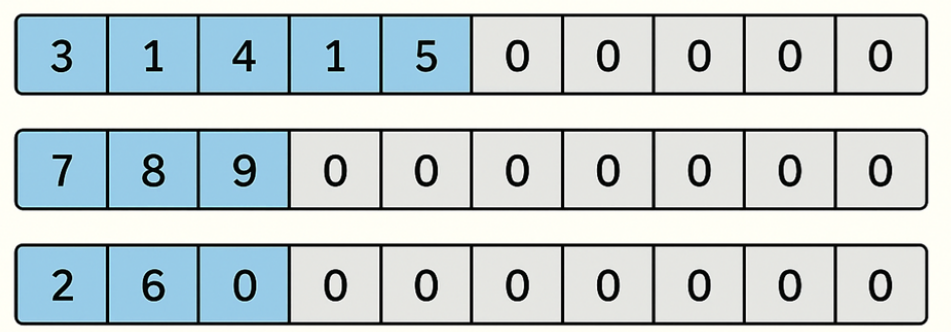
Why is Graph Deep Learning Challenging?

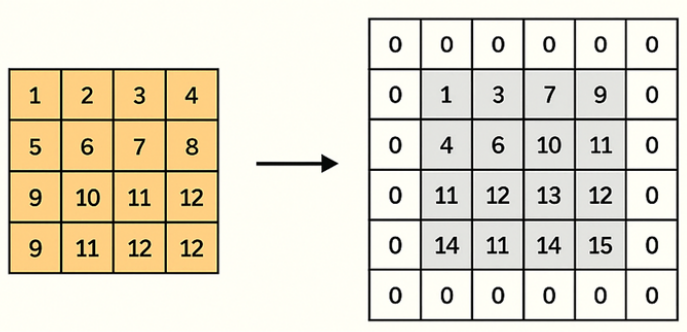
Irregular structure

Networks are inherently complex

Irregular Structure of Graphs

- Unlike images or sequences, graphs have a **highly irregular structure**.
- Traditional models like CNNs or RNNs rely on fixed input shapes (e.g., images with consistent height and width, or padded sequences).





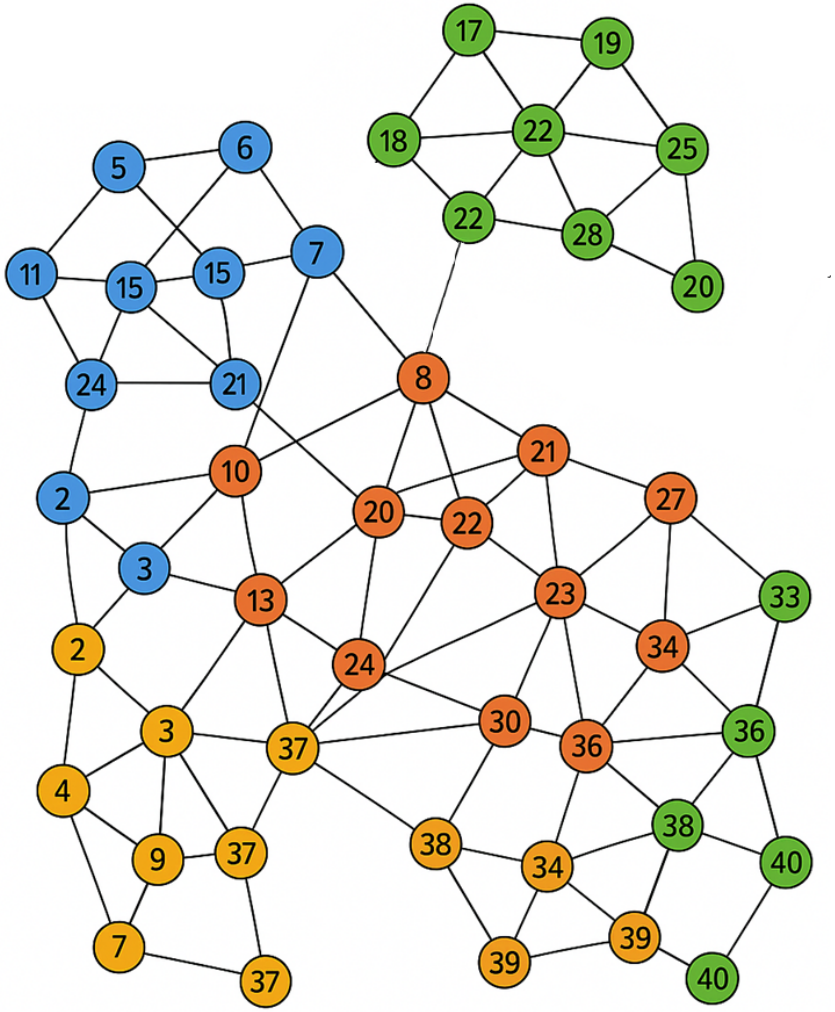
Why is Graph Deep Learning Challenging?

Irregular structure

- Graphs, however, can:
  - Vary widely in the number of **nodes**.
  - Have **nodes with varying degrees of connectivity**.

Key Implications

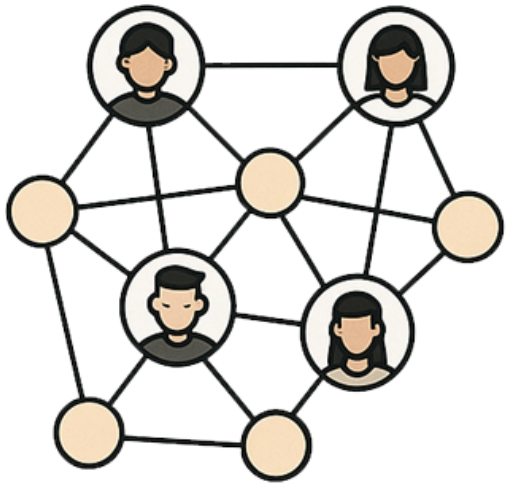
- This irregularity makes it difficult to apply standard neural operations (e.g., **convolution** or **pooling**), which assume consistent input sizes.
- Developing operations that can effectively work with these varying structures is a fundamental challenge in graph deep learning.



Why is Graph Deep Learning Challenging?

Interdependence of Data Points

- Traditional machine learning models typically assume that instances are **independent** of each other.
- However, in graph data, this assumption doesn't hold:
  - Each **node** (data point) is inherently **connected** to others.



Why This Matters

- The interconnected nature of graph data requires models that can handle these **dependencies**.
- Traditional models are not designed to account for these relationships.
- We need models that can learn from the *interactions* and *dependencies* between nodes.

Why is Graph Deep Learning Challenging?

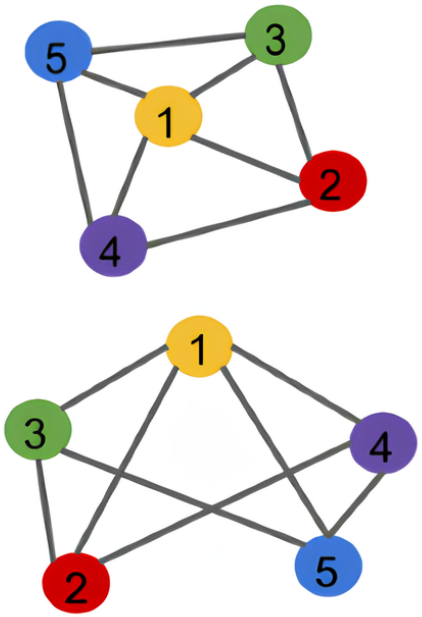
Permutation Invariance

Traditional data: fixed order

- **Images**, **text**: the order of data is meaningful
- **CNNs** and **RNNs** process data in a fixed order.

Graph data: **NO** fixed order

- In **graphs**, nodes (entities) have no inherent order.
- **Permutation invariance**: edges connect nodes, but the order of the nodes doesn't change the graph.



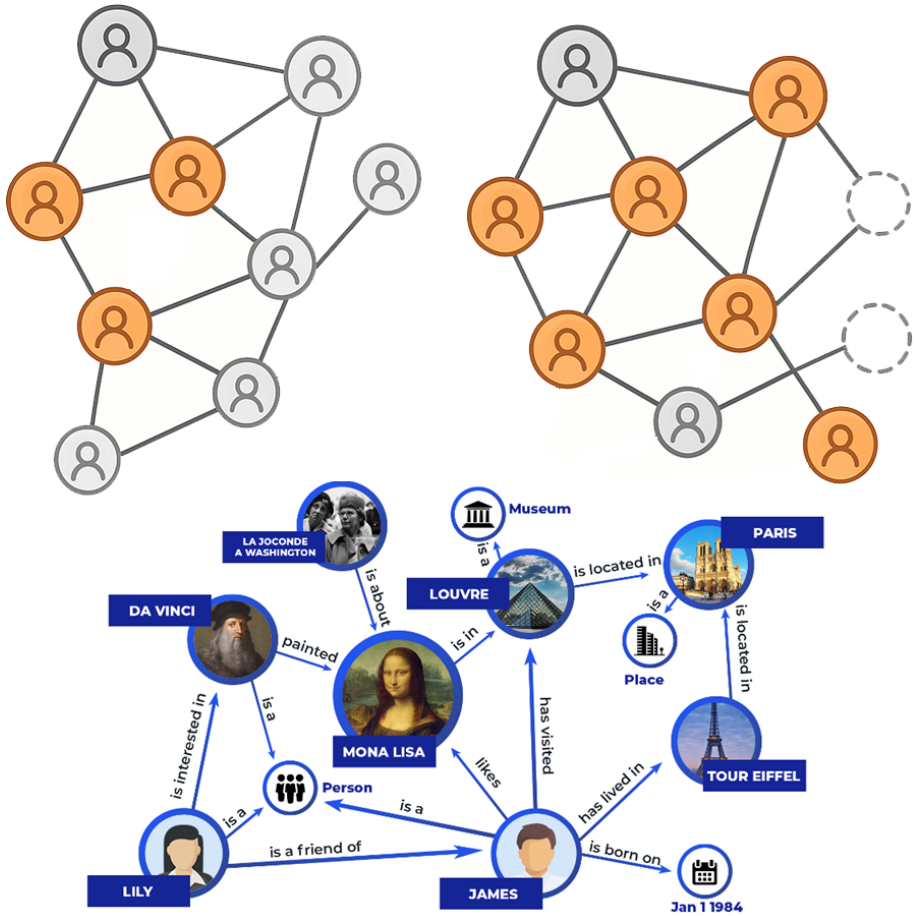
Challenges for Graph Models

- The model should give the same output regardless of the order in which nodes and edges are presented.
- Shuffling node IDs does not change the graph structure, posing challenges for traditional models that rely on fixed input structures.

Why is Graph Deep Learning Challenging?

Dynamic and Multimodal Graphs

- **Dynamic** graphs:
  - Real-world graphs are evolving over time: nodes and edges can be added, removed, or updated.
- **Multimodal** graphs:
  - Contain different types of nodes and edges
  - Different node and edge types can have various associated features, such as:
    - **User nodes** with features like age, location, interests
    - **Transaction edges** with attributes like purchase amount, time, and product type.



Basics of Deep Learning

Supervised Learning: predict an output $\boldsymbol{y}$ from an input $\boldsymbol{x}$.

- The input x can be vectors, sequences, matrices, or **graphs**.
- The task is framed as an optimization problem:

$$\min_{\theta} \mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x}))$$

- θ: a set of **parameters** we optimize
  - could contain one or more scalar, vector, matrices, etc.
- $\mathcal{L}$: **Loss Function**. Examples:
  - **L2 loss:**

$$\mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x})) := \|y - f(x)\|^2$$

  - **Cross Entropy:**

$$\mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x})) := -\sum_{i=1}^{C} y_i \log f(x)_i$$

    where $y \in \{0, 1\}^C$ is a categorical vecor (one-hot encoding).
  - Other loss function: L1 loss, max margin (hinge loss), etc.

Basics of Deep Learning

- **f** can be a simple linear layer, an MLP, CNN, or other neural networks (e.g., a GNN later).
  - A multi-layer perceptron (MLP) is a neural network composed of stacked layers:

$$f_i(\boldsymbol{x}) = \sigma(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

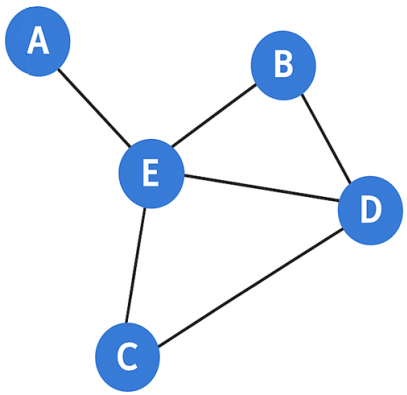
    - $\boldsymbol{W}$ and $\boldsymbol{b}$ are learnable parameters (weights and biases).
    - σ is the activation function (e.g., ReLU, Sigmoid).
- **Optimization**: We solve the optimization problem using gradients:

$$\theta \leftarrow \theta - \eta \nabla_\theta \mathcal{L}$$

  - η is the learning rate.
  - $\boldsymbol{\nabla_\theta \mathcal{L}} \rightarrow$ directional derivative in the direction of largest increase
  - Use stochastic gradient descent (SGD) to optimize $\mathcal{L}$ for weights θ over many iterations.
  - Other higher order optimisers: RMSprop, Adam, Adagrad, etc.

Setup

- Assume we have a graph $G = (V, E)$, where:
  - $V \rightarrow$ the set of graph nodes $V = \{v_1, ..., v_N\}$, $N =$ num. nodes
  - $E \rightarrow$ the edge set, each edge defined as (v_i, v_j)
- $X = [x_1, ..., x_N] \rightarrow$ node feature set, $X \in \mathbb{R}^{NxD}$, $D =$ dimension of x_i
- $A \in \mathbb{R}^{NxN} \rightarrow$ adjacency matrix:
  - binary: $1's$ and $0's$
  - weighted: each edge has a strength $e_{ij} \in R$:
    - $e_{ij} > 0$, if $(v_i, v_j) \in E$
    - $e_{ij} = 0$, if $(v_i, v_j) \notin E$
- $D_{ii} = \sum_j A_{ij}$ degree matrix



Graph G

	A	B	C	D	E
A	0	0	0	0	1
B	0	0	0	1	1
C	0	0	0	1	1
D	0	1	1	0	0
E	1	1	1	1	0

Adjacency matrix A

	A	B	C	D	E
A	1	0	0	0	0
B	0	2	0	0	0
C	0	0	2	0	0
D	0	0	0	3	0
E	0	0	0	0	4

Degree matrix D

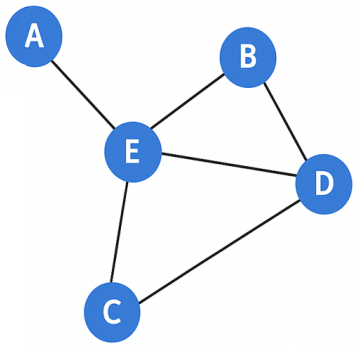
A	-1.1	3.2	4.3
B	0.2	6.1	-1.3
C	1.2	1.3	1.4
D	-1.4	4.3	3.1
E	1.3	2.8	4.2

Feature vector X

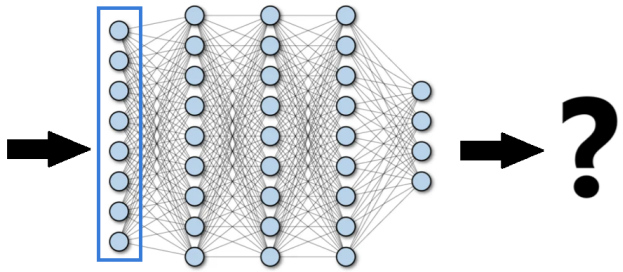
How Can We Apply Neural Networks to Graphs?

Naive Approach for Graph Representation

- Join the *adjacency matrix* and *node features*
- Feed them into a deep neural network.



	A	B	C	D	E	Feat		
A	0	0	0	0	**1**	-1.1	3.2	4.3
B	0	0	0	**1**	**1**	0.2	6.1	-1.3
C	0	0	0	**1**	**1**	1.2	1.3	1.4
D	0	**1**	**1**	0	0	-1.4	4.3	3.1
E	**1**	**1**	**1**	**1**	0	1.3	2.8	4.2



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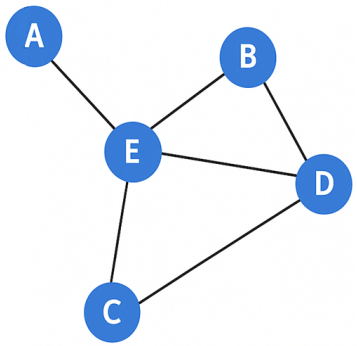
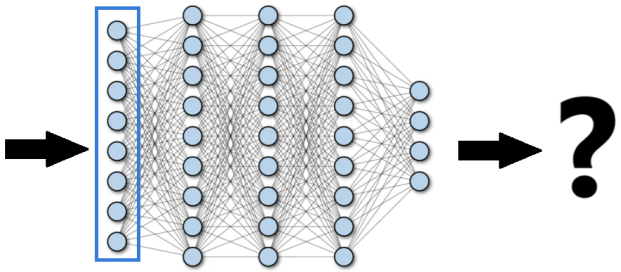


	A	B	C	D	E	Feat		
A	0	0	0	0	1	-1.1	3.2	4.3
B	0	0	0	1	1	0.2	6.1	-1.3
C	0	0	0	1	1	1.2	1.3	1.4
D	0	1	1	0	0	-1.4	4.3	3.1
E	1	1	1	1	0	1.3	2.8	4.2

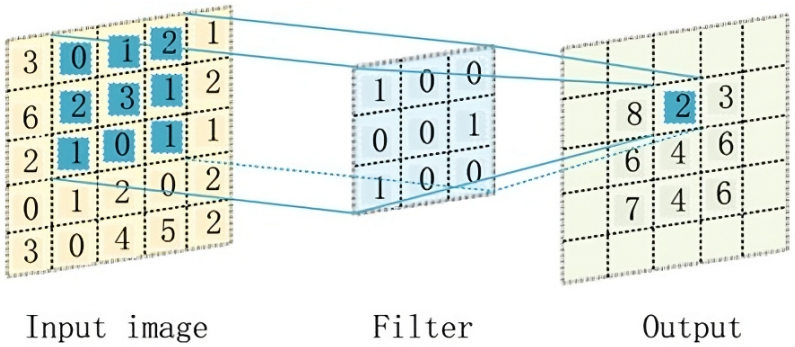


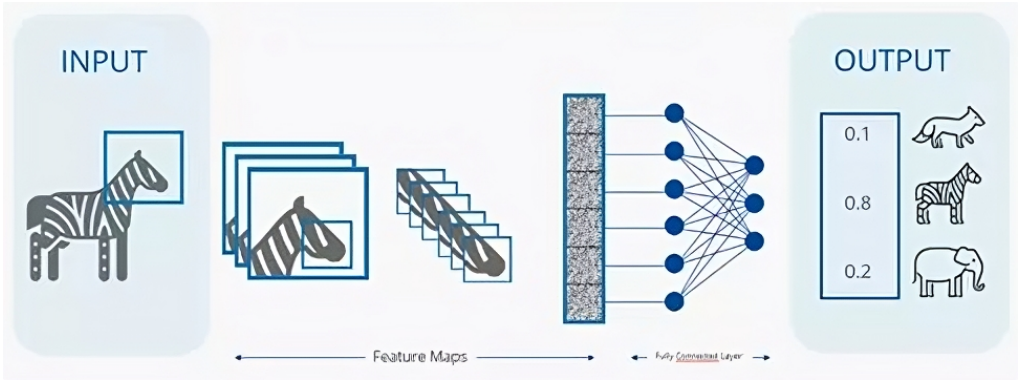
Problems with This Approach

- $O(|V|)$ parameters
- Not applicable to graphs of different sizes.
- Sensitive to node ordering.

How Can We Apply Neural Networks to Graphs?

Idea: Convolutional Networks





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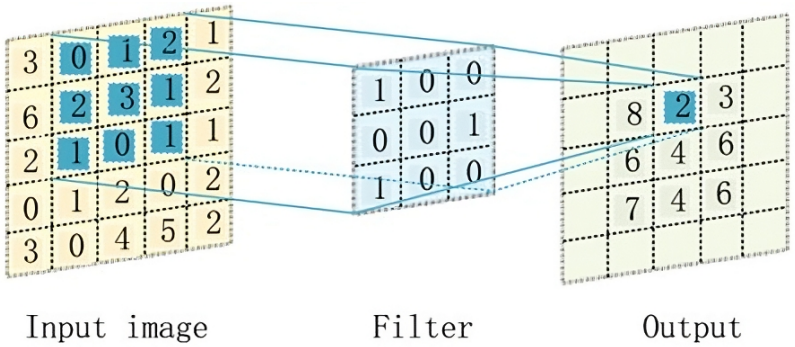
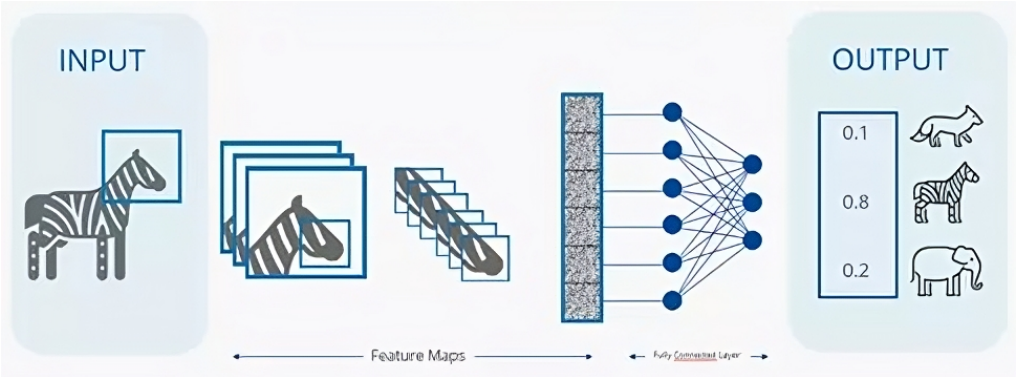
Idea: Convolutional Networks





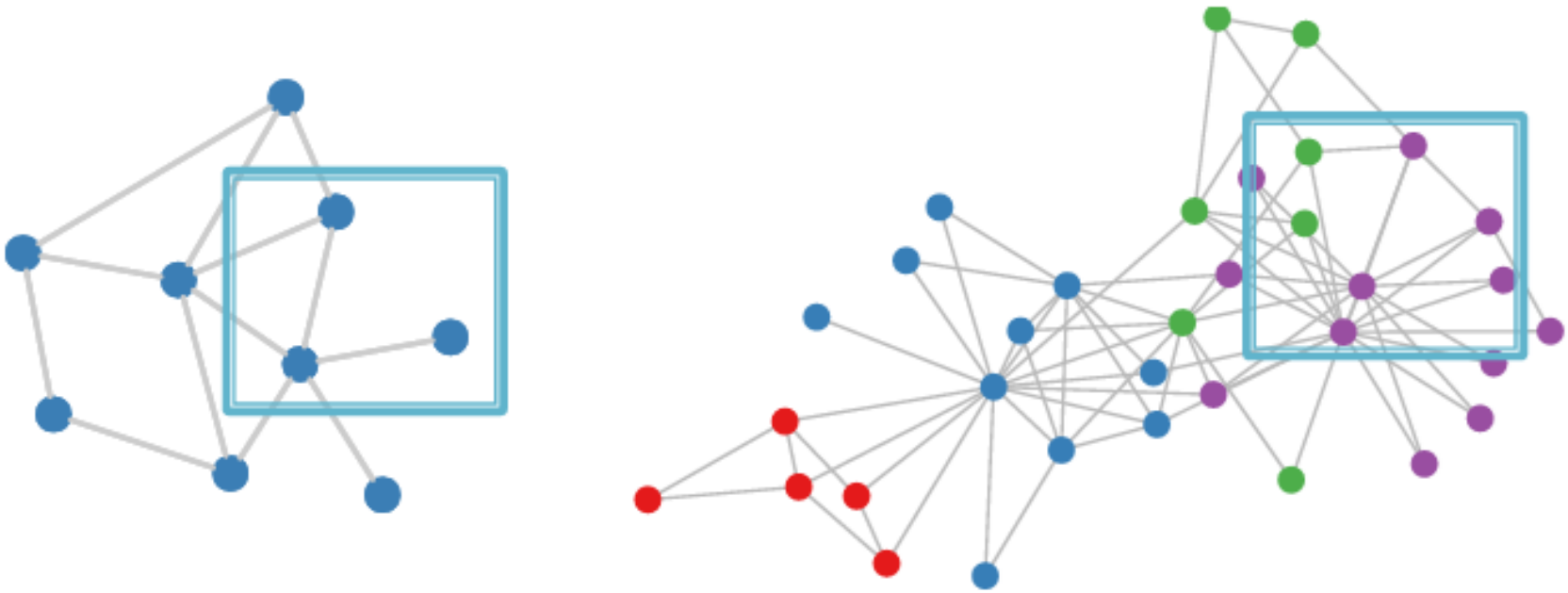
Goals

- Generalize convolutions beyond simple lattices
- Leverage node features/attributes.

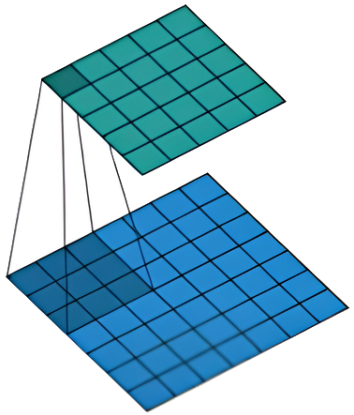
From Images to Graphs

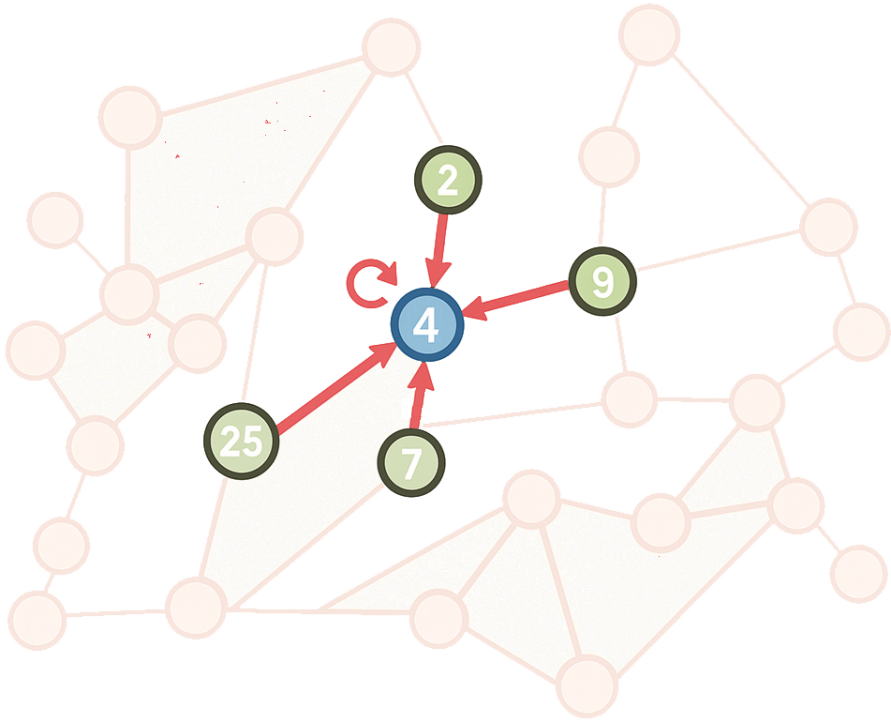
What if Our Data Looks Like This?

- *Graph-structured data* lacks a fixed notion of locality.
- There's no *sliding window* over graphs.
- Graphs are **permutation-invariant**.



From Images to Graphs





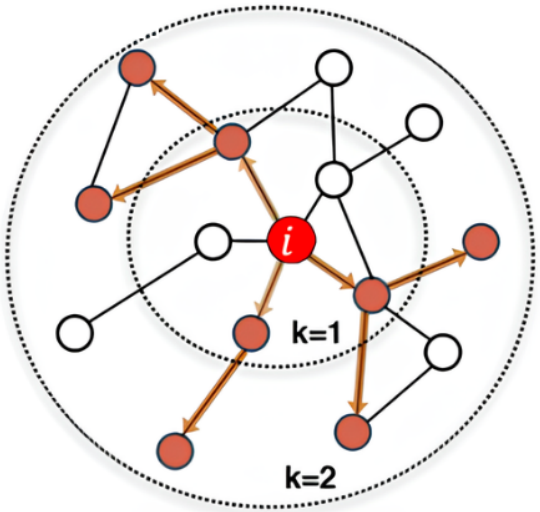
Idea

- **Transform** neighbor information and **combine** it:
  - Transform *messages* h_i from neighbors: $W_i h_i$
  - Sum them up: $\sum_i W_i h_i$

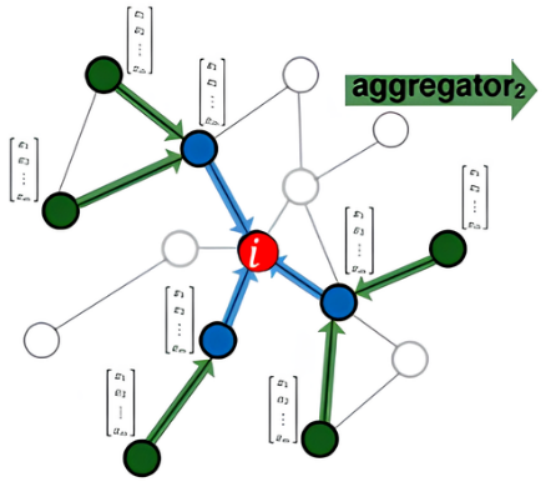
Graph Neural Networks

Key Ideas

- The neighborhood of a node defines a **computation graph**
- Learn how to **propagate** information across the graph to compute node features



Determine node computation graph

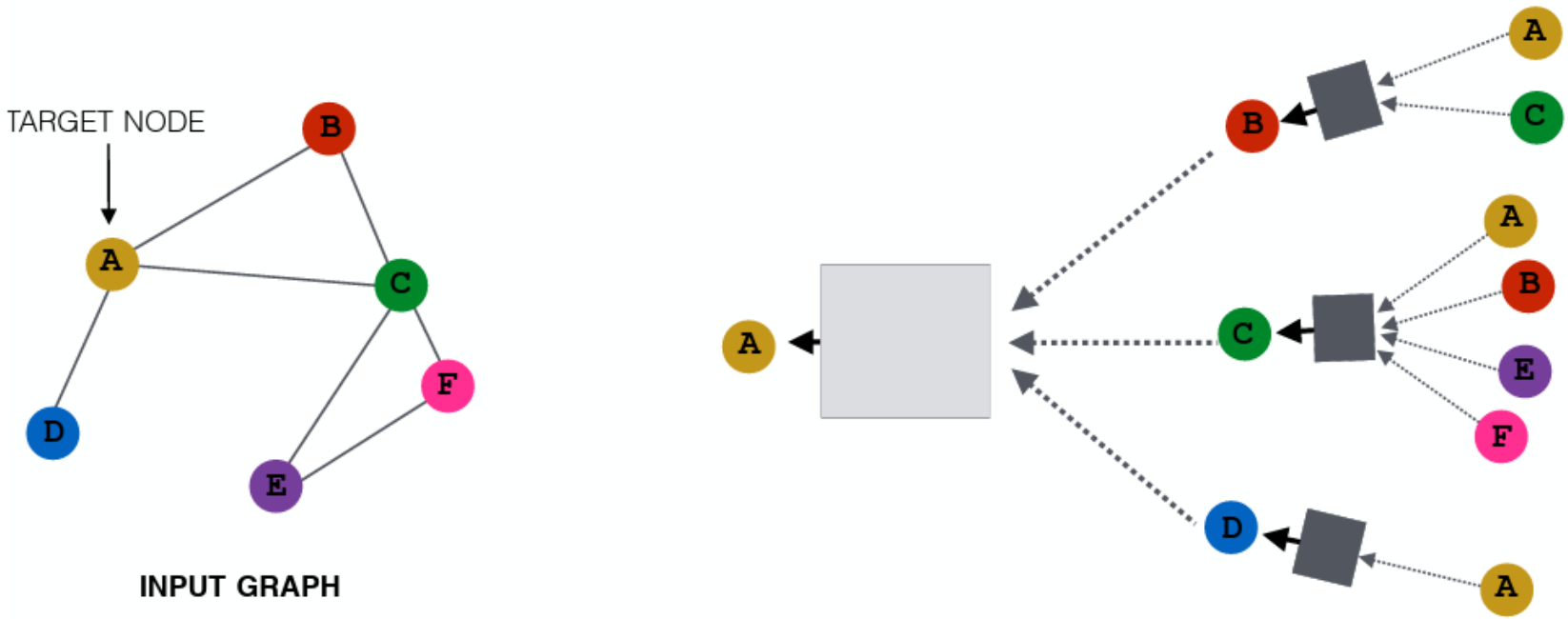


Propagate and transform information

Idea: Aggregating Information from Neighbors

Key Idea

- Generate node embeddings based on **local network neighborhoods**



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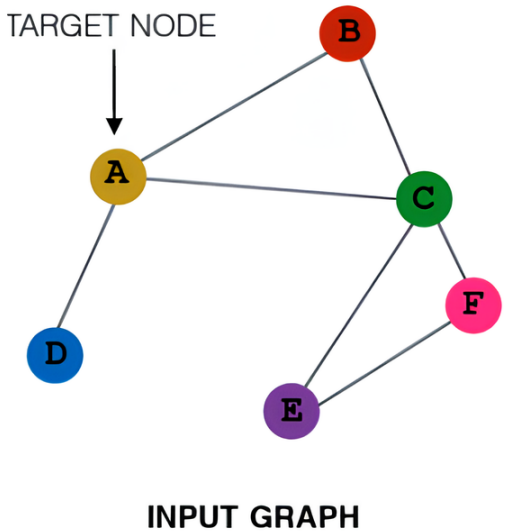
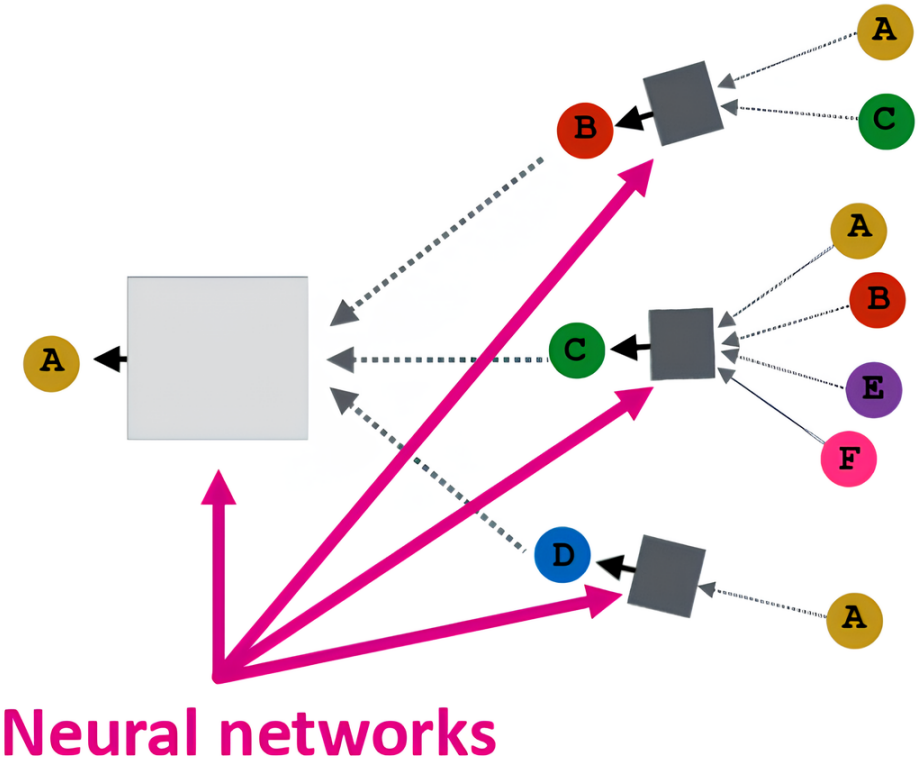
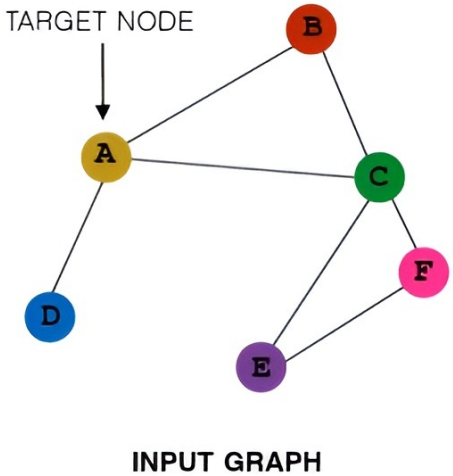
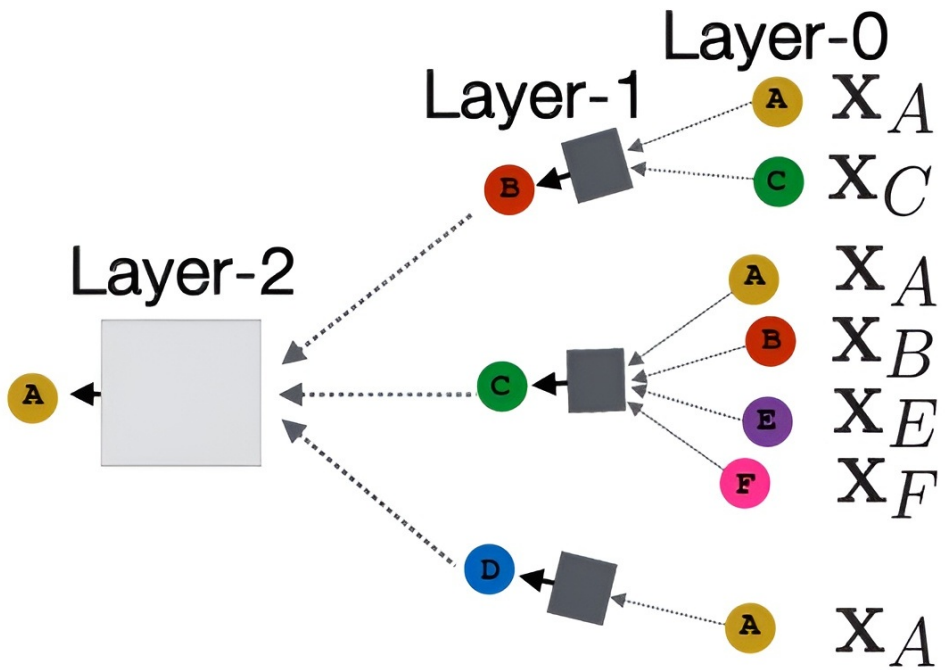




Network Depth

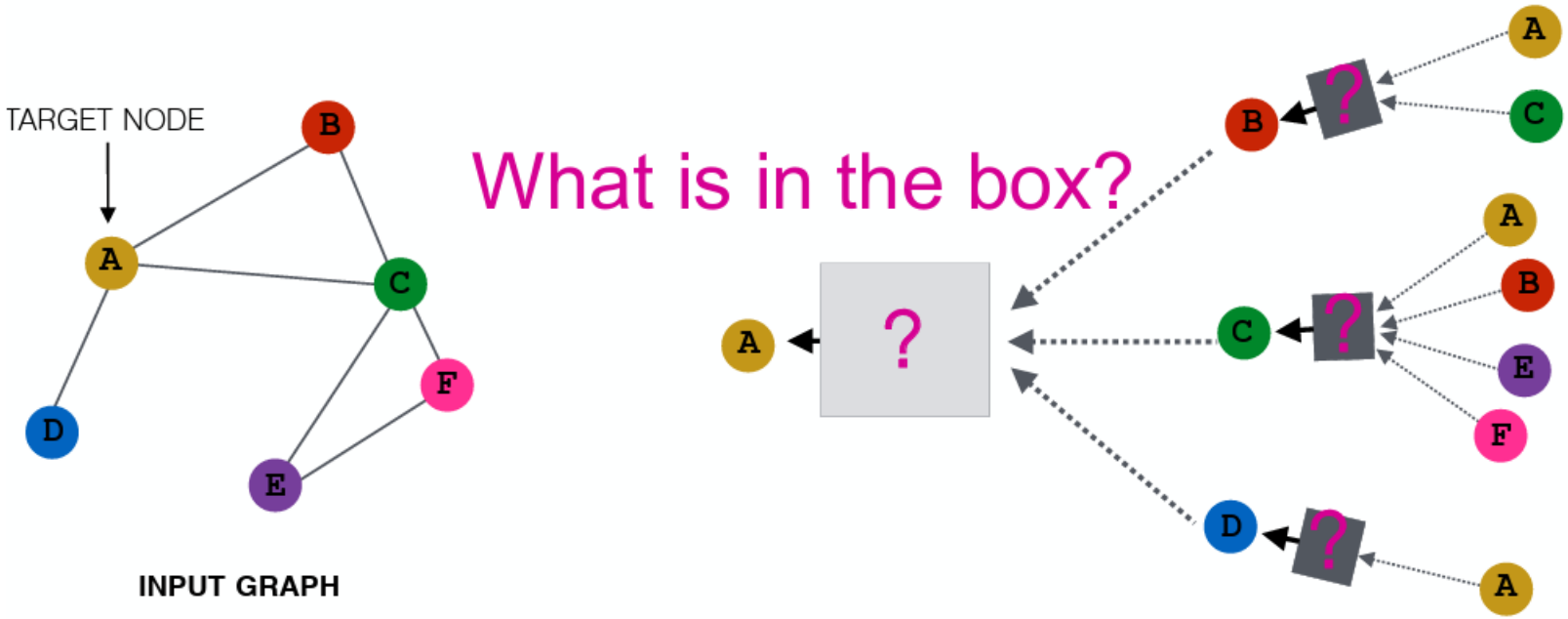
- The network can have an arbitrary depth.
- At each layer, nodes have **embeddings** (features).
- **Layer 0**: embedding of node v is its input feature x_v.
- **Layer-k**: embeddings h_v contain information from nodes that are K hops away in the graph.





Neighborhood Aggregation

Key distinction between GNNs: How different approaches aggregate information across layers.



Neighborhood Aggregation

Basic approach?

Neighborhood Aggregation

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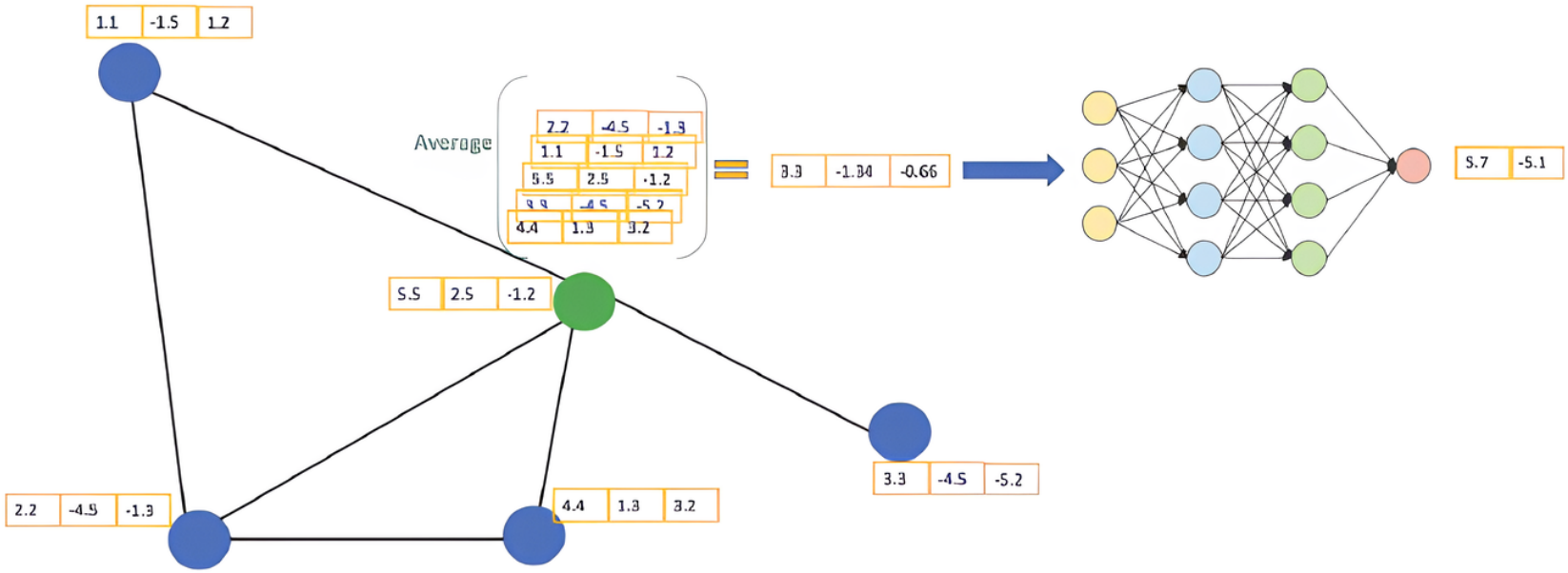
Average information from neighbors and apply a neural network.



Graph Deep Encoder: The Math

Basic approach?

Average information from neighbors and apply a **neural network**.

$h_v^{(0)} = x_v$ ← Initial 0-th layer embeddings are equal to node features

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Average information from neighbors and apply a **neural network**.

$h_v^{(0)} = x_v$ ← Initial 0-th layer embeddings are equal to node features

$$h_v^{(k+1)} = \sigma\left(W_k^{(0)} h_v^{(k)} + W_k^{(1)} \sum_{u \in N(v)} \frac{h_u^{(k)}}{|N(v)|}\right), \forall k \in \{0, \ldots, K-1\}$$

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Embedding of v at layer k

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Average of neighbor's previous layer embeddings

Graph Deep Encoder: The Math

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$h_v^{(0)} = x_v$ ← Initial 0-th layer embeddings are equal to node features

Non-linearity (e.g., ReLU) → σ

Embedding of v at layer k → $h_v^{(k)}$

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Average of neighbor's previous layer embeddings → $\sum_{u \in N(v)} \frac{h_u^{(k)}}{|N(v)|}$

Graph Deep Encoder: The Math

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$$h_v^{(0)} = x_v$$

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Average of neighbor's previous layer embeddings

Number of layers

$z_v = h_v^{(K)}$ ← Embedding after K layers of neighborhood aggregation

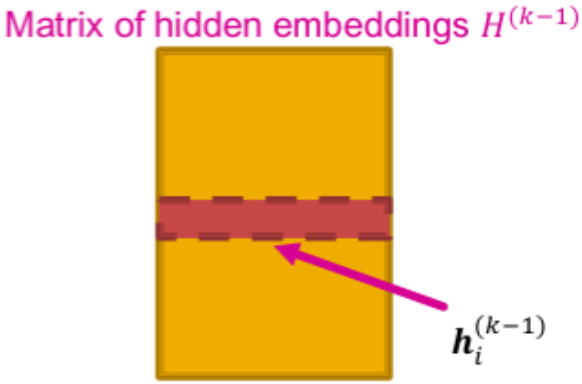
Efficient Aggregation Using Matrix Operations

Many aggregations can be performed efficiently by (sparse) matrix operations

Let $H^{(k)} = [h_1^{(k)} \quad h_2^{(k)} \quad \dots \quad h_{|V|}^{(k)}]^T$

Then the node feature aggregation can be written as:

$$\sum_{v \in N(u)} h_v^{(k)} = A_{:,v} H^{(k)}$$



Let D be the diagonal degree matrix:

$$D_{v,v} = \text{Deg}(v) = |N(v)|$$

Note: The inverse of D is also diagonal.

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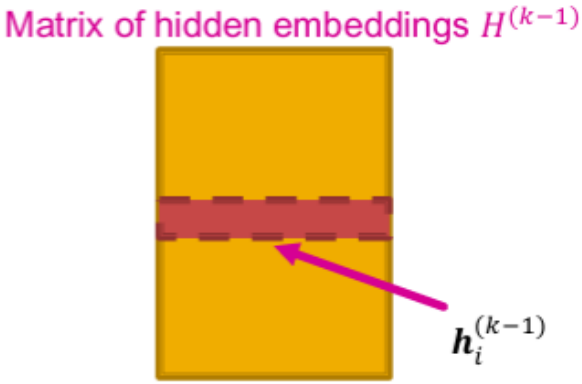

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Therefore:

$$\sum_{u \in N(v)} \frac{h_u^{(k)}}{|N(v)|} \Longrightarrow \boldsymbol{H^{(k+1)} = D^{-1} A H^{(k)}}$$

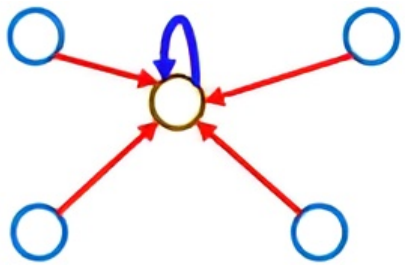
GNN Update Rule: Matrix Form

Update Equation

$$H^{(k+1)} = \sigma\left(\tilde{A}H^{(k)}W_k^{(1)^T} + H^{(k)}W_k^{(0)^T}\right)$$

where

- $\tilde{A} = D^{-1}A$: normalized adjacency matrix
- $H^{(k)} = [h_1^{(k)} \dots h_{|V|}^{(k)}]^\top$: node features at layer k



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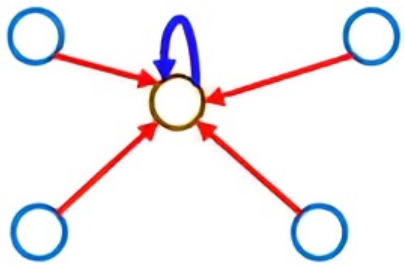


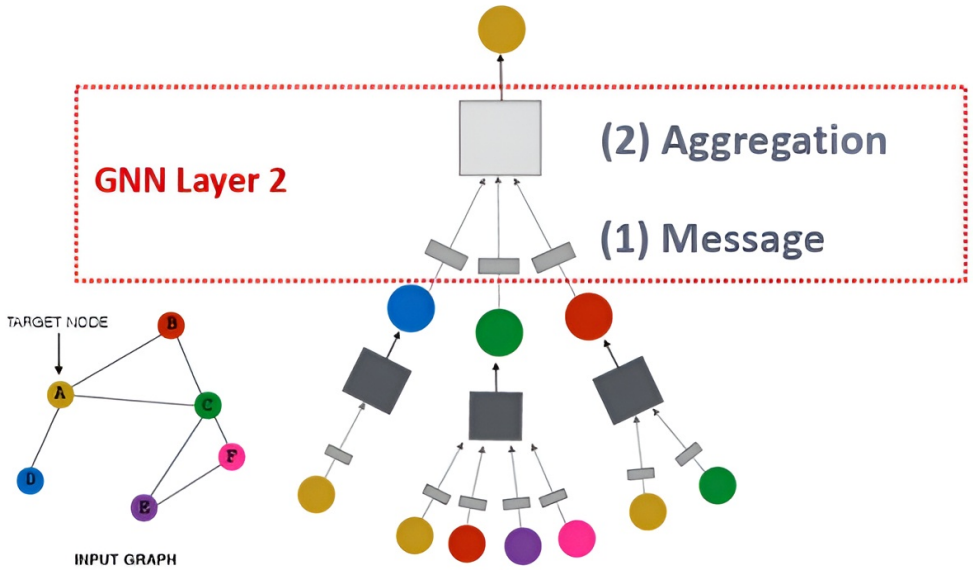
Efficiency Note

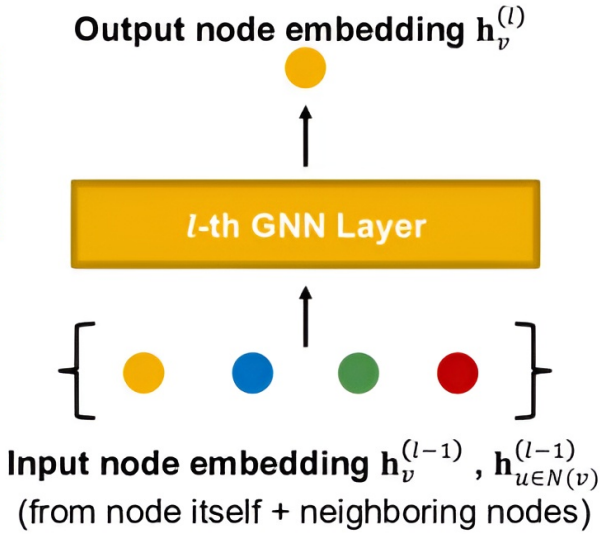
A is sparse $\Rightarrow$ enables efficient sparse matrix multiplication

A Single GNN Layer

Key Idea

- Compress a set of vectors into a single vector
- **GNN Layer = Message + Aggregation**





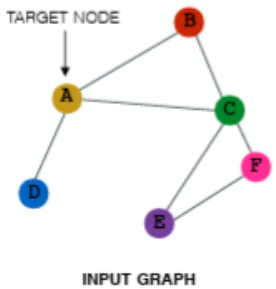
A Single GNN Layer: Message Computation

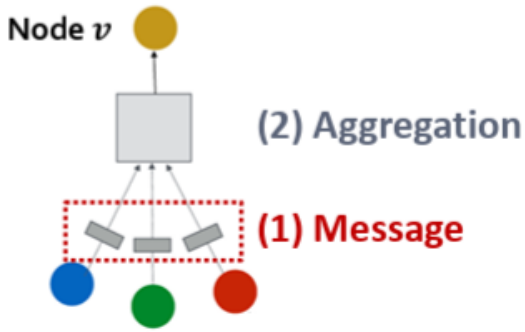
Message Computation

$$\mathbf{m}_u^{(k)} = \text{MSG}^{(k)}(\mathbf{h}_u^{(k-1)})$$

- **Intuition:** Each node creates a message to be sent to its neighbors.
- **Example:** Linear transformation

$$\mathbf{m}_u^{(k)} = \boldsymbol{W}_1^{(k)} \mathbf{h}_u^{(k-1)}$$





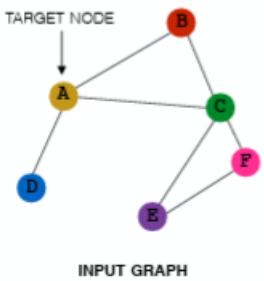
A Single GNN Layer: Aggregation

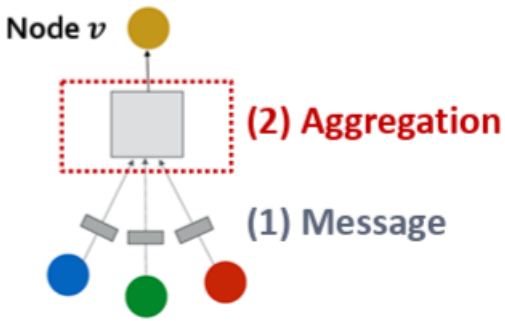
Aggregation

$$\mathbf{h}_v^{(k)} = \text{AGG}^{(k)}\left(\left\{\mathbf{m}_u^{(k)} \mid u \in \mathcal{N}(v)\right\}\right)$$

- **Intuition:** Node v aggregates messages from its neighbors $u \in \mathcal{N}(v)$
- **Examples of AGG:** `sum()`, `mean()`, or `max()`
- **Example:**

$$\mathbf{h}_v^{(k)} = \sum_{u \in \mathcal{N}(v)} \mathbf{m}_u^{(k)}$$





A Single GNN Layer: Aggregation Issue and Solution

Issue: Node's Own Information May Be Lost

- Aggregation only over neighbors: $\mathbf{h}_v^{(k)} = \text{AGG}^{(k)}\left(\left\{\mathbf{m}_u^{(k)} \mid u \in \mathcal{N}(v)\right\}\right)$
- **Problem:** $\mathbf{h}_v^{(k)}$ does not directly depend on node v's own features.

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- **Problem:** $\mathbf{h}_v^{(k)}$ does not directly depend on node v's own features.

Solution: Include Self-Messages

- **(1) Message from node v itself:** $\mathbf{m}_v^{(k)} = \boldsymbol{W}_{\mathbf{0}}^{(k)}\mathbf{h}_v^{(k-1)}$
  (separate from $\boldsymbol{W}_{\mathbf{1}}^{(k)}$ used for neighbors)
- **(2) Aggregation:**
  - First aggregate from neighbors:

$$\mathbf{h}_{\mathcal{N}(v)}^{(k)} = \text{AGG}^{(k)}\left(\left\{\mathbf{m}_u^{(k)} \mid u \in \mathcal{N}(v)\right\}\right)$$

  - Then combine with self-message:

$$\mathbf{h}_v^{(k)} = \text{CONCAT}\left(\mathbf{h}_{\mathcal{N}(v)}^{(k)}, \mathbf{m}_v^{(k)}\right)$$

Classical GNN Layers: GCN

Graph Convolutional Network (GCN) Update Rule

$$\mathbf{h}_v^{(k)} = \sigma\left(\sum_{u \in \mathcal{N}(v) \cup \{v\}} \frac{1}{\sqrt{d_u d_v}} \boldsymbol{W}^{(k)} \mathbf{h}_u^{(k-1)}\right)$$

- **Message:**

$$\mathbf{m}_u^{(k)} = \boldsymbol{W}^{(k)} \mathbf{h}_u^{(k-1)}$$

  Each neighbor (and the node itself) sends a message using shared weight matrix $\boldsymbol{W}^{(k)}$.

- **Aggregation:**
  - Normalize messages by node degrees d_u, d_v
  - Sum messages from neighbors **and the node itself**
  - Apply non-linearity σ (e.g., ReLU)
- **Note:** The input graph is assumed to include self-loops.

This formulation is from Kipf & Welling (2017).

Classical GNN Layers: GraphSAGE

GraphSAGE Update Rule

$$\mathbf{h}_v^{(k)} = \sigma\left(\boldsymbol{W}^{(k)} \cdot \text{CONCAT}\left(\mathbf{h}_v^{(k-1)}, \text{AGG}^{(k)}\left(\left\{\mathbf{h}_u^{(k-1)} \mid u \in \mathcal{N}(v)\right\}\right)\right)\right)$$

Two-Stage Aggregation

- **Stage 1: Neighborhood Aggregation**

$$\mathbf{h}_{\mathcal{N}(v)}^{(k)} = \text{AGG}^{(k)}\left(\left\{\mathbf{h}_u^{(k-1)} \mid u \in \mathcal{N}(v)\right\}\right)$$

- **Stage 2: Combine with Node Itself**

$$\mathbf{h}_v^{(k)} = \sigma\left(\boldsymbol{W}^{(k)} \cdot \text{CONCAT}\left(\mathbf{h}_v^{(k-1)}, \mathbf{h}_{\mathcal{N}(v)}^{(k)}\right)\right)$$

This formulation is from Hamilton et al., (2017).
It formulation supports inductive learning on unseen graphs.

Classical GNN Layers: GraphSAGE Neighbor Aggregation

- **Mean**: Take an average of neighbor features

$$\text{AGG}^{(k)} = \underbrace{\sum_{u \in \mathcal{N}(v)} \frac{\mathbf{h}_u^{(k-1)}}{|\mathcal{N}(v)|}}_{\text{Aggregation} \quad \text{Message Computation (Identity)}}$$

- **Pool**: Apply transformation before aggregation (e.g., MLP)

$$\text{AGG}^{(k)} = \underbrace{\text{Mean}\left(\left\{\text{MLP}^{(k)}(\mathbf{h}_u^{(k-1)}) \mid u \in \mathcal{N}(v)\right\}\right)}_{\text{Aggregation} \quad \text{Message Computation}}$$

- **LSTM**: Order-sensitive aggregation over neighbors

$$\text{AGG}^{(k)} = \underbrace{\text{LSTM}^{(k)}\left(\left[\mathbf{h}_u^{(k-1)} \mid u \in \pi(\mathcal{N}(v))\right]\right)}_{\text{Aggregation (learned over sequence)}}$$

Questions?