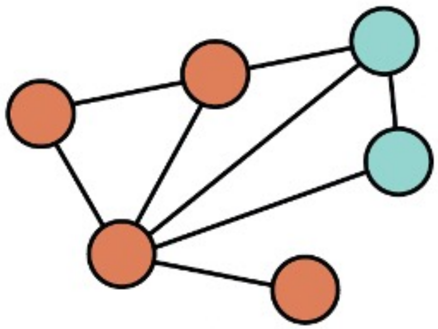
BOSTON UNIVERSITY



Graph Neural Networks

DL4DS – Spring 2025

April Dates

Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	Saturday
	April 1	2	3	4 **GANs**	5	6
7	8	9 **VAEs**	10 **Discussion**	11 **Diffusion Models**	12	13
14	15	16 **Graph Neural Nets (VizWiz Leaders Share)**	17 **Discussion**	18 **Reinforcement Learning**	19	20
21	22	23 **TBD/Overflow (JEPA Models)**	24 **Discussion**	25 **★ Project Presentations 1 ★**	26	27
28	29	30 **★ Project Presentations 2 ★**	May 1 **Discussion??**	2 Study Period	3 Study Period	4
5	6 Final Exams	7 Final report & Repo **	8	9	10	11

** Might be earlier. Depends on when grades are due.

Project Presentations

Format:
$\leq$ 3 minutes screencast/video
$\leq$ 2 minutes additional presentation
~2 minutes Q&A

Will post slot assignments tonight!!
Final project info updated on Gradescope and website.

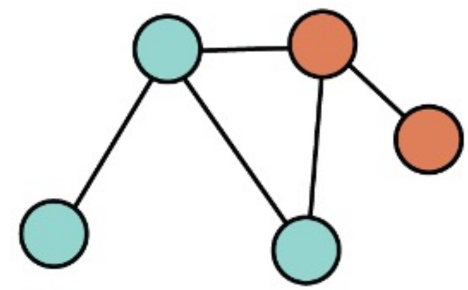
April 25 – 75 minutes

- Slot 1
- Slot 2
- Slot 3
- Slot 4
- Slot 5
- Slot 6
- Slot 7
- Slot 8

April 30 – 75 minutes

- Slot 9
- Slot 10
- Slot 11
- Slot 12
- Slot 13
- Slot 14
- Slot 15
- Slot 16
- Slot 17

Graph Neural Networks



Neural architectures that process graphs.

Three challenges:

1. Variable topology
2. Size (billions of nodes)
3. Single monolithic graph

Topics

- Basic definition and examples
- Graph representation
- Properties of Adjacency Matrix
- Graph neural network, tasks and loss functions
- Graph convolutional network
- Graph & Node classification
- Edge graphs

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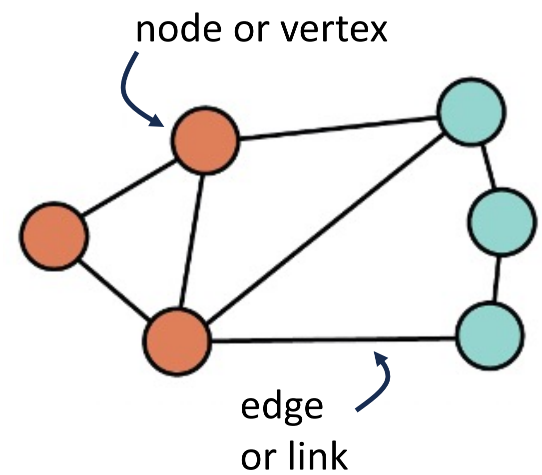
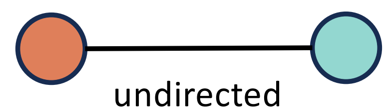
Graph (Network)

- general structure composed of *nodes* (vertices) and *edges* (links)

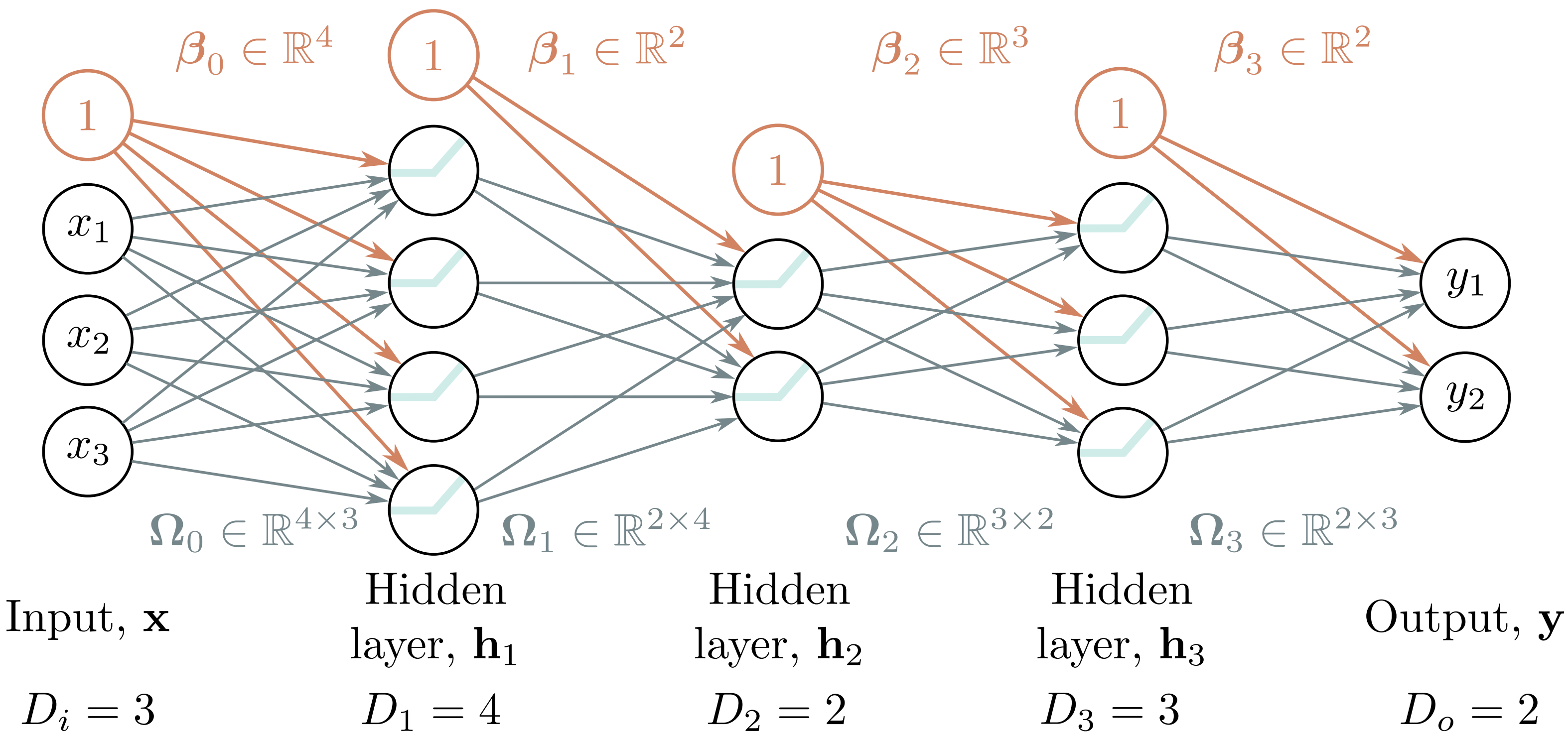
- edges can be *undirected* or *directed*

- a graph with directed edges and no cycles (no loops) is called *directed acyclic graph* (DAG)

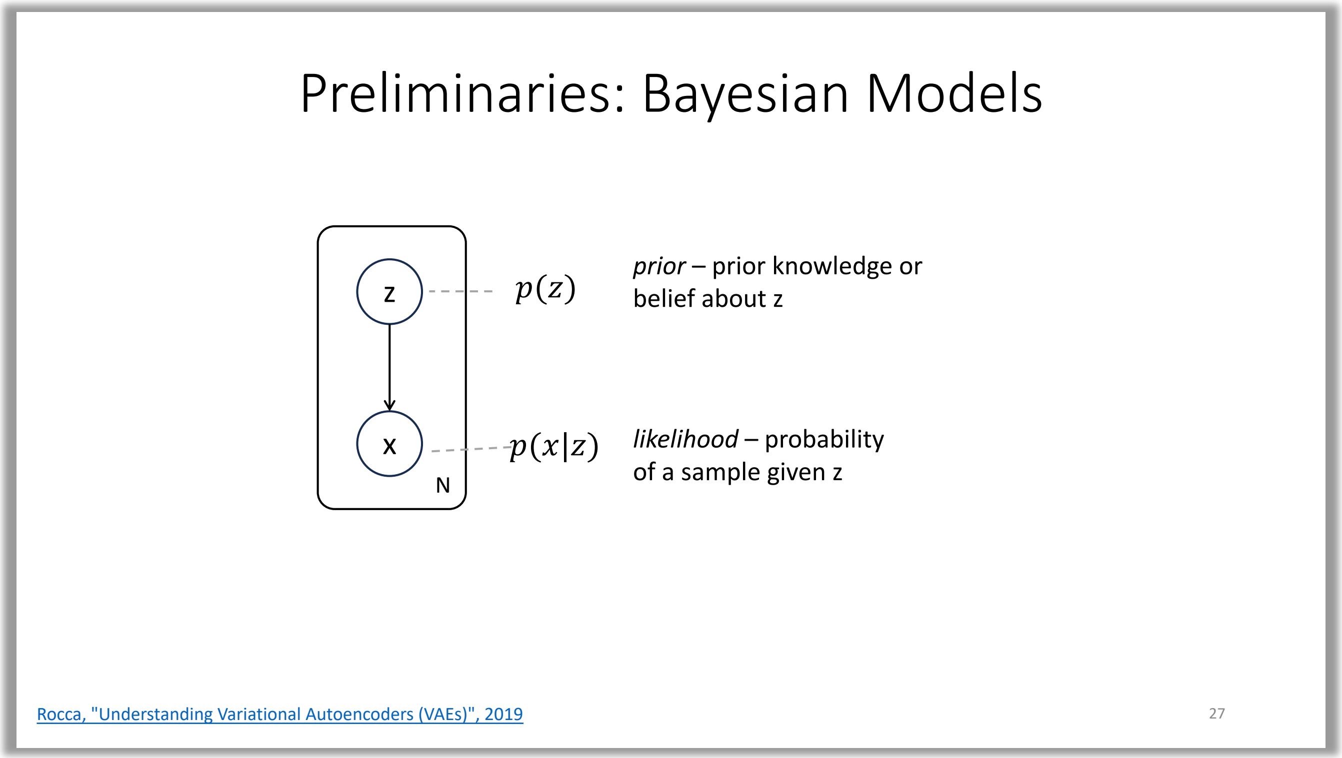




Directed Example – Feed Forward Network

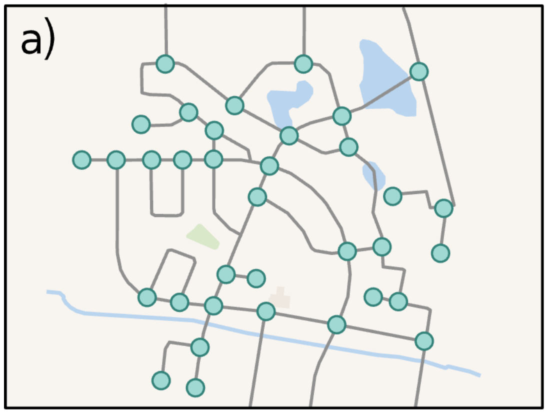


Directed Example – Bayesian Graphical Model

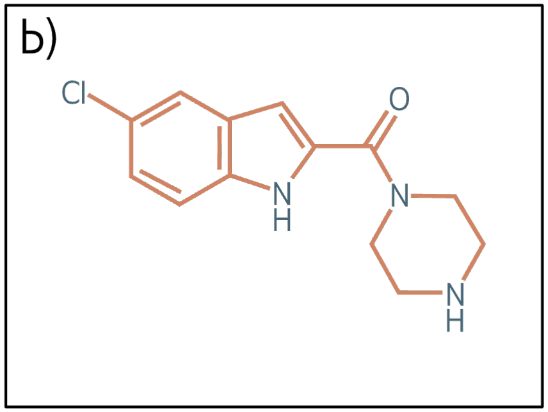


From lecture 18 – Variational Autoencoders

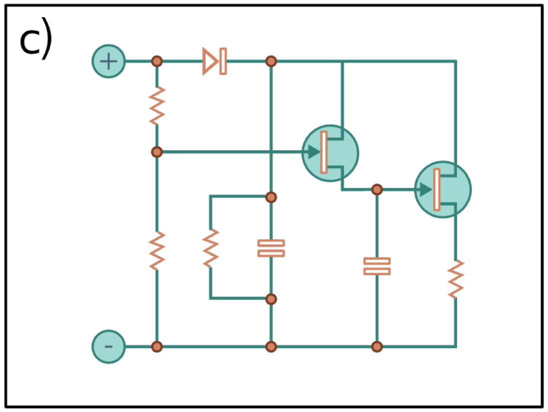
Undirected Examples



road networks
nodes: physical locations or landmarks
edges: connecting roads

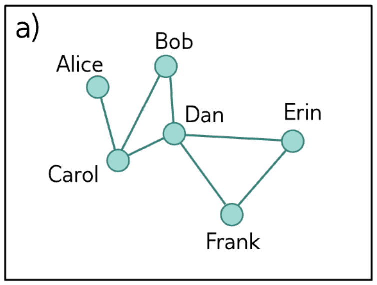


chemical molecules
nodes: atoms
edges: chemical bonds

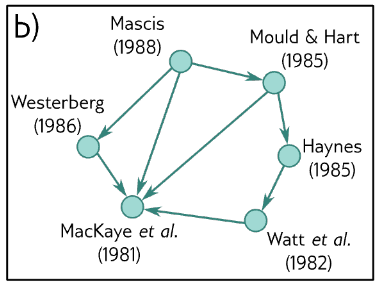


electrical circuits
nodes: components or junctions
edges: wires/electrical connections

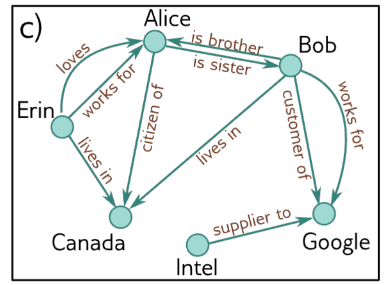
Examples



social networks
nodes: people
edges: friendships
(undirected)

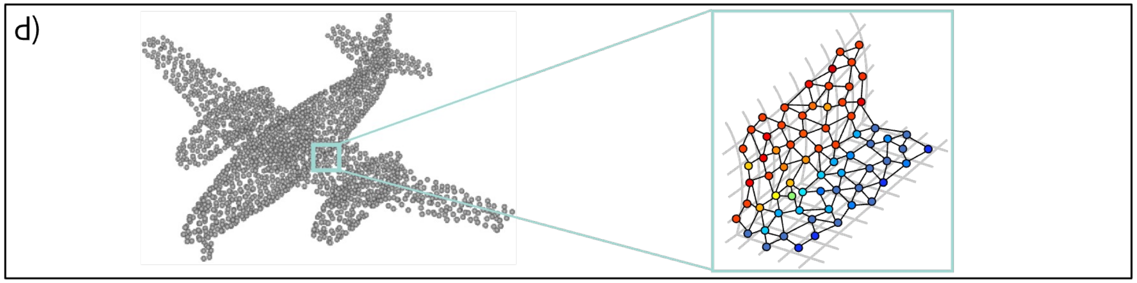


science literature
nodes: papers
edges: citations
(acyclic directed)



knowledge graph
nodes: objects
edges: named relationship
(cyclic directed)

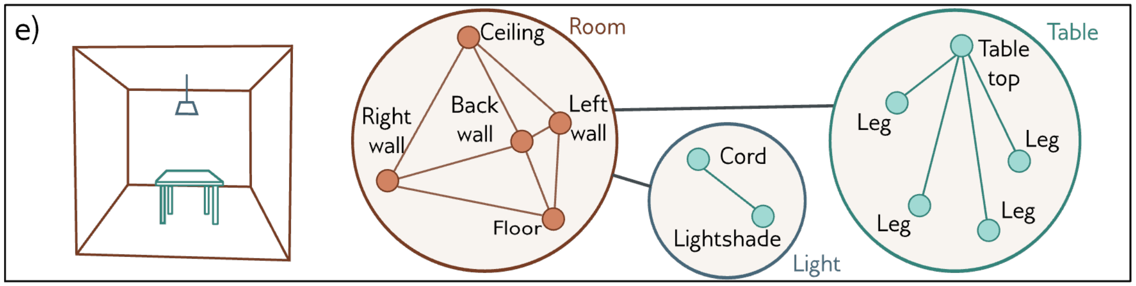
Example – Geometric Point Cloud



nodes: positions in 3D space (vertex in 3D graphics)
edges: connections to nearby points
(undirected)

https://en.wikipedia.org/wiki/Vertex_(computer_graphics)

Example – Scene Graph



hierarchical graph showing relationship between objects in a 3D scene

nodes: composite graphs or objects in 3D space
edges: connections to nearby points
(undirected)

Fernandez-Madrigal and Gonzalez, "Multi-hierarchical graph search," 2002
Armeni et al, “3D Scene Graph: A structure for unified semantics, 3D space and camera,” 2020?
Wald et al, “Learning 3D Semantic Scene Graphs with Instance Embeddings,” 2022

Other examples

- Wikipedia – nodes are articles, edges are hyperlinks between articles
- Computer programs – nodes are syntax tokens, edges are computation between tokens (tensor graph from Gradients lecture)
- Protein interactions – nodes are proteins, edges exist where two proteins interface
- Set or list – every element is connected to every other element
- image – each pixel is a node with edges to the eight adjacent pixels

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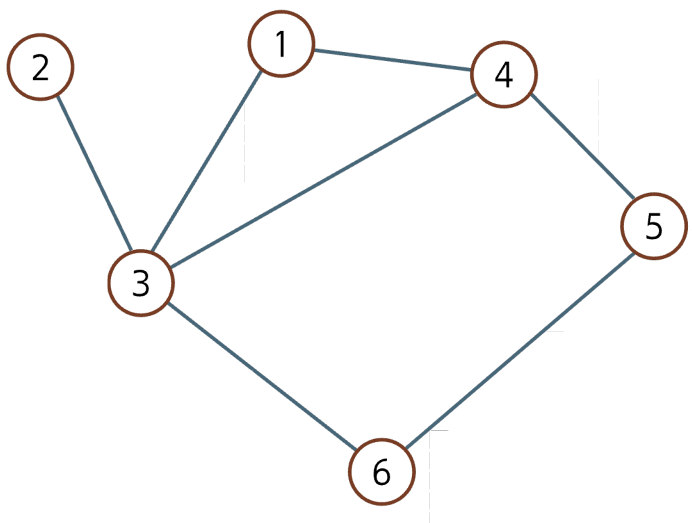
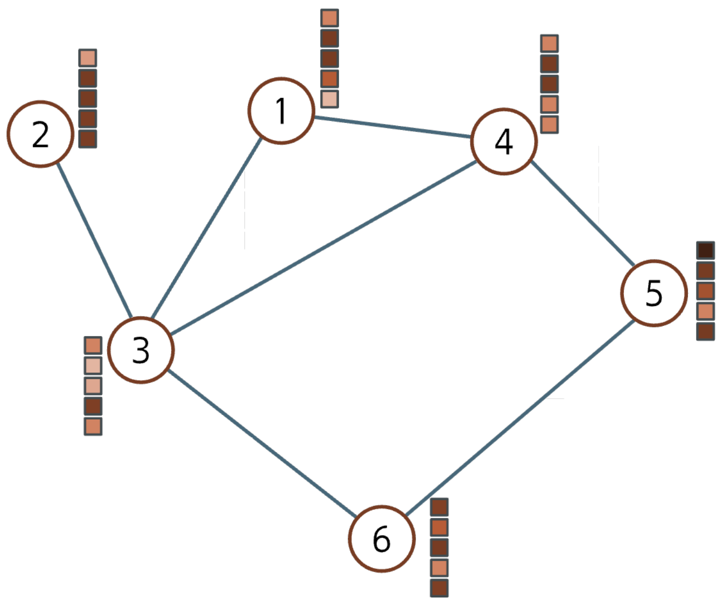
Graph representation



Example undirected graph with 6 nodes

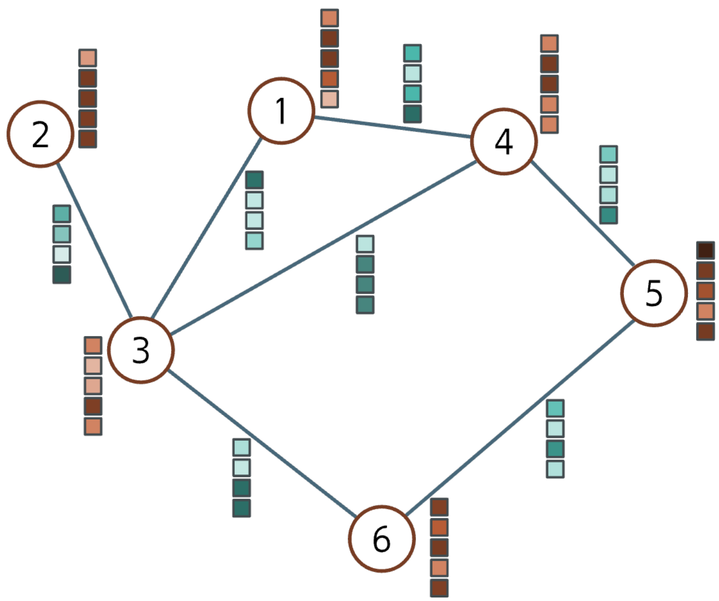
Graph representation – node embedding



Example undirected graph with 6 nodes

Information about a node is stored in a *node embedding*

Graph representation – edge embedding

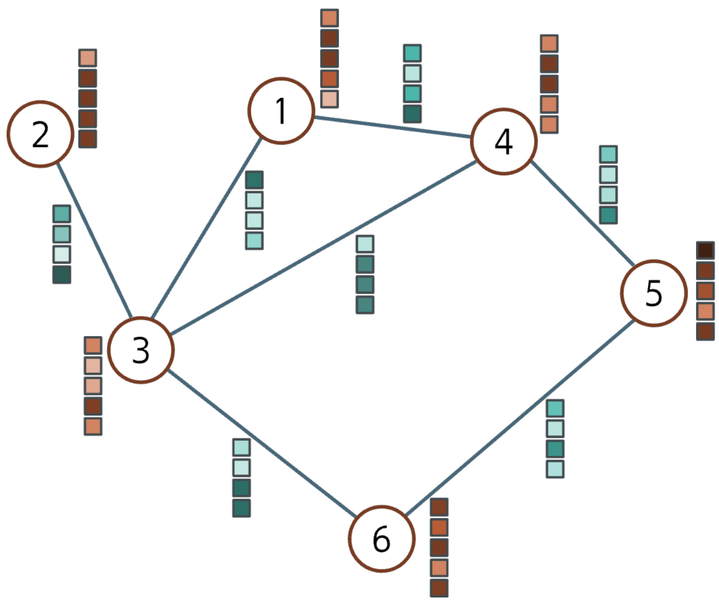


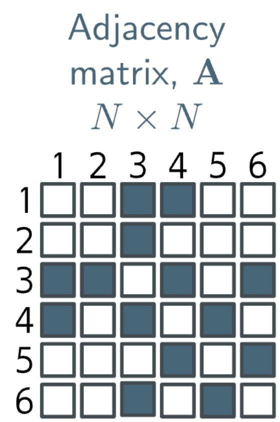
Example undirected graph with 6 nodes

Information about a node is stored in a *node embedding*

Information about an edge is stored in an *edge embedding*

Graph representation – adjacency matrix





Assume we have N nodes

The graph connections can be represented by an *adjacency matrix*

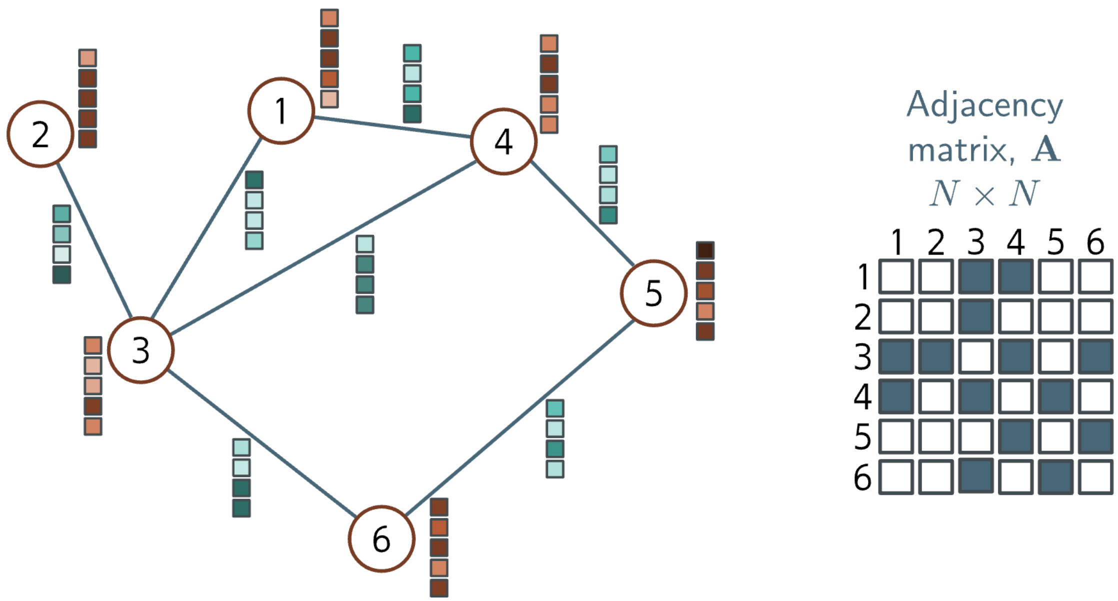
Where a value of 1 at (m, n) represents a connection between nodes m and n.

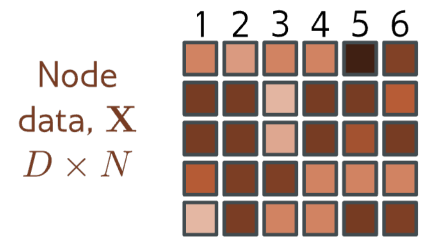
For undirected graphs the matrix is always symmetric about the diagonal

Diagonal is zero – no edge to itself

Can be very sparse

Graph representation – node data matrix



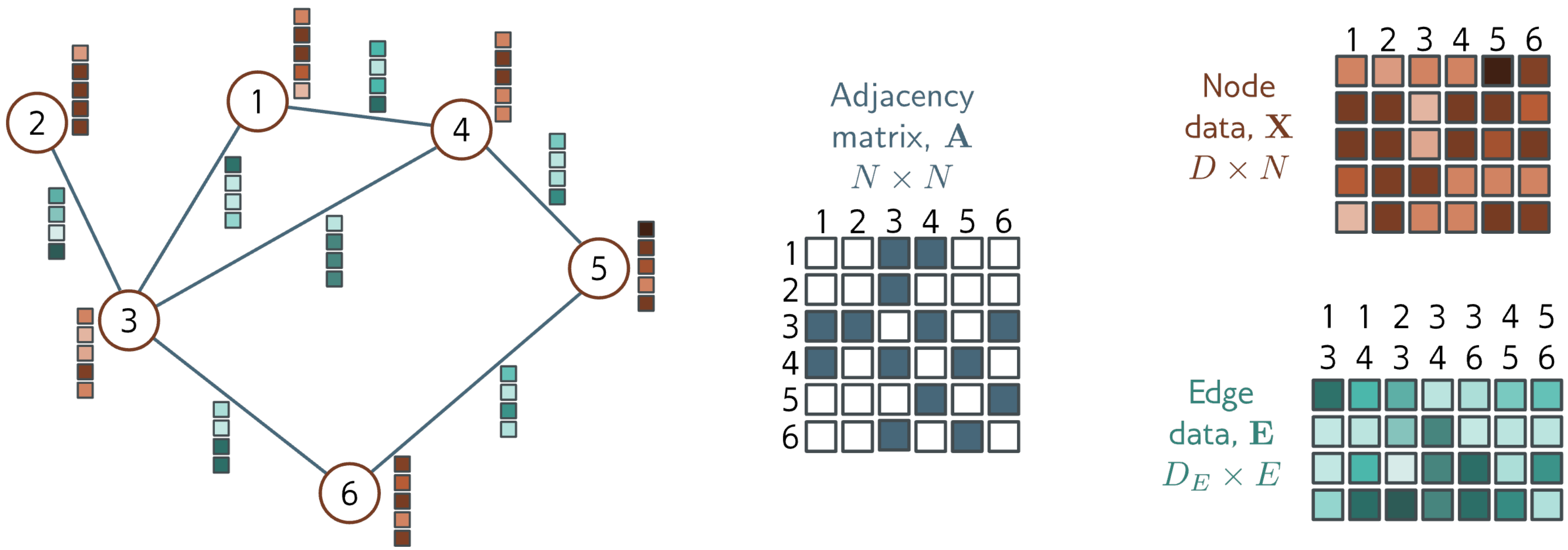


All the node data in the form of node embeddings can represented by a *Node data matrix*

Where D is the dimension of the note embedding and

N is the number of nodes

Graph representation – edge data matrix



Similarly, all the edge embedding information can be stored in an *Edge data matrix*, where:
D_E is the dimension of the edge embedding vector and
E is the number of edges

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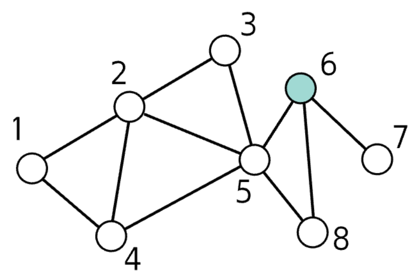
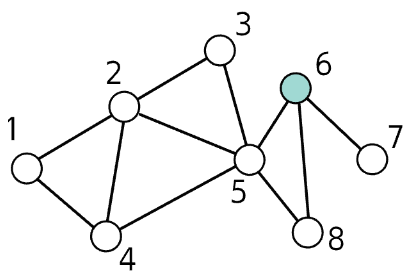
Adjacency Matrix



Assume we have an 8-node undirected graph

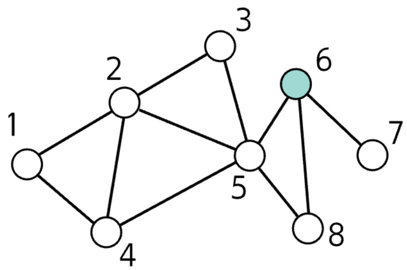
Adjacency Matrix



$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

Adjacency matrix for this graph.

Adjacency Matrix



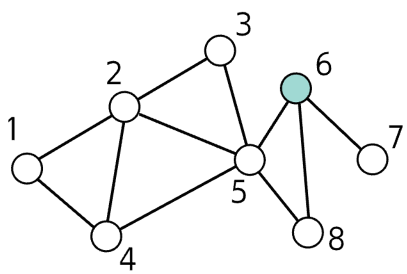
$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

adjacency matrix

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

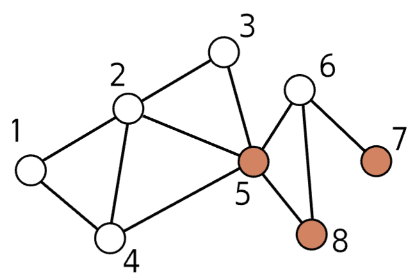
We can one hot encode representation of node 6

Adjacency Matrix



$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

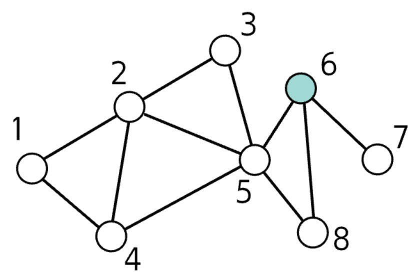
$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \qquad \mathbf{Ax} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$



If we pre-multiply the one-hot encoded data node vector x by adjacency matrix A we get the 6th column of A indicating direct connections to other nodes

One-hot encoding vector of all nodes directly connected node 6

Adjacency Matrix

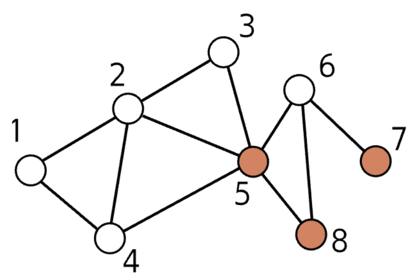


$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

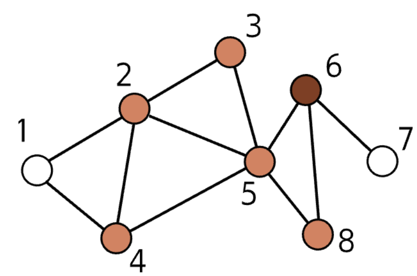
If we pre-multiply again by A, we get a vector showing the number of times we can get to each node in 2 steps.

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\mathbf{Ax} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$



$$\mathbf{A}^2\mathbf{x} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \\ 1 \\ 3 \\ 0 \\ 1 \end{bmatrix}$$

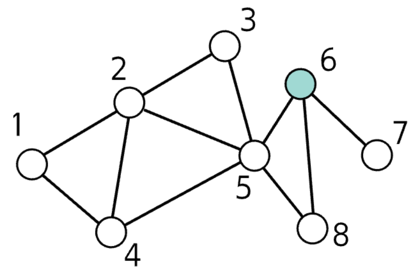


Graph showing all nodes that can be reached in *exactly* 2 steps.

Adjacency Matrix

Pre-multiplying x by A twice is equivalent to the matrix A^2

Shows how many times you can get from node m to node n in 2 steps

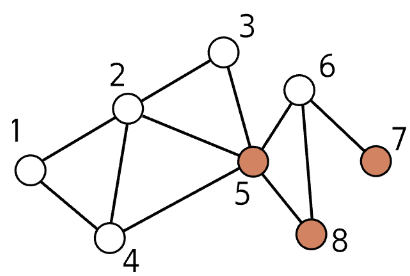


$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

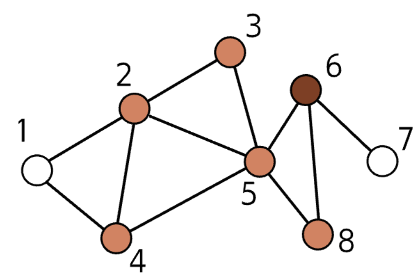
$$\boxed{\mathbf{A}^2 = \begin{bmatrix} 2 & 1 & 1 & 1 & 2 & 0 & 0 & 0 \\ 1 & 4 & 1 & 2 & 2 & 1 & 0 & 1 \\ 1 & 1 & 2 & 2 & 1 & 1 & 0 & 1 \\ 1 & 2 & 2 & 3 & 1 & 1 & 0 & 1 \\ 2 & 2 & 1 & 1 & 5 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 3 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 & 2 \end{bmatrix}}$$

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

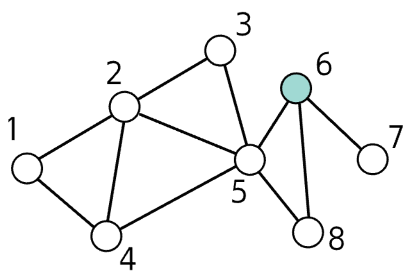
$$\mathbf{Ax} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$



$$\mathbf{A}^2\mathbf{x} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \\ 1 \\ 3 \\ 0 \\ 1 \end{bmatrix}$$



Adjacency Matrix



$$\mathbf{A}^2 = \begin{bmatrix} 2 & 1 & 1 & 1 & 2 & 0 & 0 & 0 \\ 1 & 4 & 1 & 2 & 2 & 1 & 0 & 1 \\ 1 & 1 & 2 & 2 & 1 & 1 & 0 & 1 \\ 1 & 2 & 2 & 3 & 1 & 1 & 0 & 1 \\ 2 & 2 & 1 & 1 & 5 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 3 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 & 2 \end{bmatrix}$$

Example for $L = 2$

When you raise the adjacency matrix to the power of L,

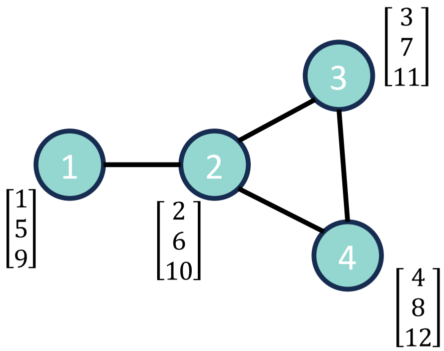
the entry at position (m, n) of $\mathbf{A}^L$ contains the number of unique walks of length L from node n to node m

Note: this is not the same as the number of unique paths since it includes routes that visit the same node more than once.

a non-zero entry at position (m, n) indicates that the distance from m to n must be less than or equal to L.

Permutation of node indices

Since node indexing is arbitrary, we can permute the node indices



$$\begin{array}{cc} & \begin{matrix}(1 & 2 & 3 & 4)\end{matrix} \\ \mathbf{X} = & \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix} \end{array}$$

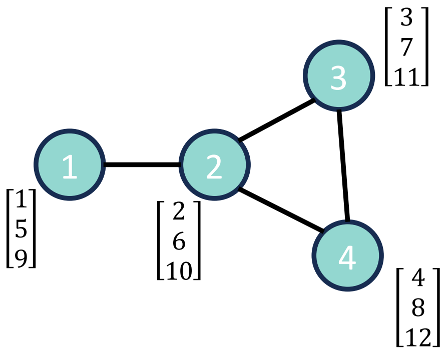
node data

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

adjacency matrix

Permutation of node indices

Since node indexing is arbitrary, we can permute the node indices



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node data

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

adjacency matrix

$$\begin{array}{cc} & \begin{matrix}(3 & 4 & 2 & 1)\end{matrix} \\ \mathbf{P} = & \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \end{array}$$

We can express this mathematically with a permutation matrix, $\mathbf{P}$

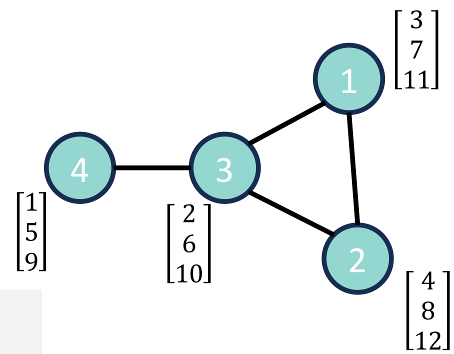
New: $(1 \quad 2 \quad 3 \quad 4)$
Old: $(3 \quad 4 \quad 2 \quad 1)$

$$\mathbf{X}' = \mathbf{XP} = \begin{bmatrix} 3 & 4 & 2 & 1 \\ 7 & 8 & 6 & 5 \\ 11 & 12 & 10 & 9 \end{bmatrix}$$

Permute the columns of the Node data matrix

$$\mathbf{A}' = \mathbf{P}^{\mathrm{T}}\mathbf{AP} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Permute both the rows and column of the Adjacency matrix



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Graph Neural Network

- A graph neural network is a model that takes the node embeddings $\mathbf{X}$ and the adjacency matrix $\mathbf{A}$ as inputs and passes them through a series of K layers.
- The node embeddings are updated at each layer to create intermediate "hidden" representations $\mathbf{H}_K$ before finally computing output embeddings $\mathbf{H}_K$.
- At the start of this network, each column of the input node embeddings $\mathbf{X}$ just contains information about the node itself.
- At the end, each column of the model output $\mathbf{H}_K$ includes information about the node and its context within the graph.
- This is like word embeddings passing through a transformer network. These represent words at the start but represent the word meanings in the context of the sentence at the end.

Graph Level Tasks

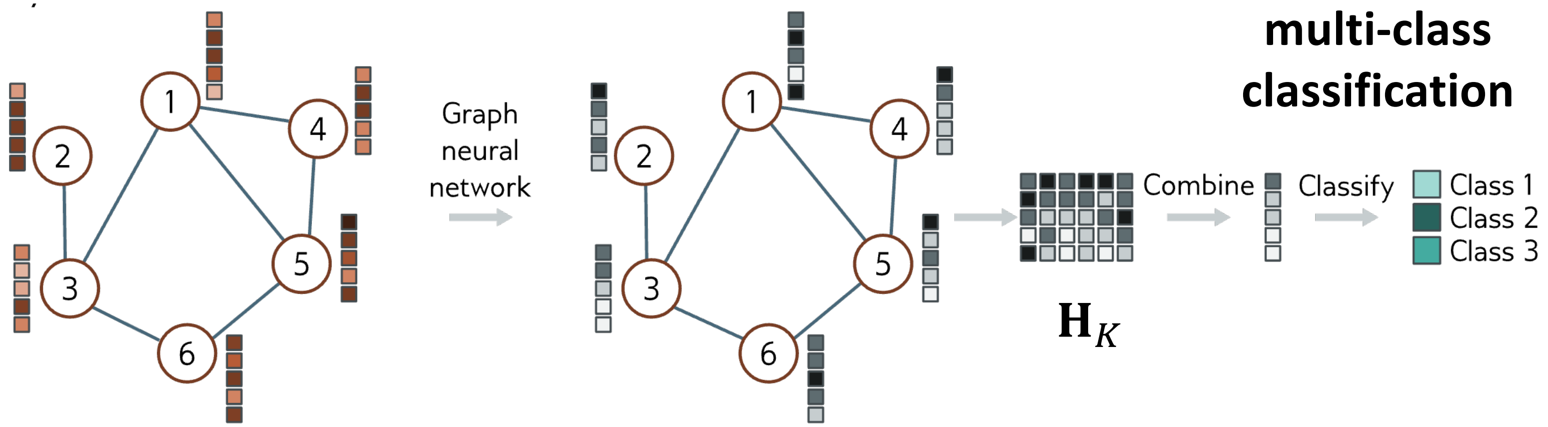
Determine

- class categories, e.g. molecule is poisonous
- regression values, e.g. molecure boiling and freezing point

based on graph structure and node embeddings

For graph-level tasks, the output node embeddings are combined (e.g., by averaging), and the resulting vector is mapped via a linear transformation or neural network to a fixed-size vector

Graph level classification



Binary Classification: $\mathrm{Pr}(y = 1|\mathbf{X}, \mathbf{A}) = \mathrm{sigmoid}[\beta_K + \underbrace{\omega_K \mathbf{H}_K \mathbf{1} \; /N}_{\text{Mean pooling}}]$

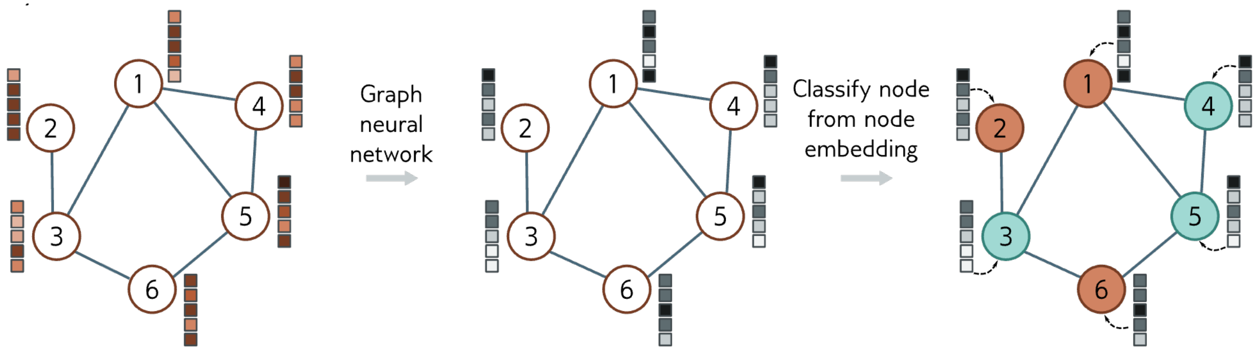
β_K is scalar

ω_K is $1 \times D$ row vector

$\mathbf{H}_K$ is the output embedding matrix

$\mathbf{1}$ is the output embedding matrix

Node level binary classification

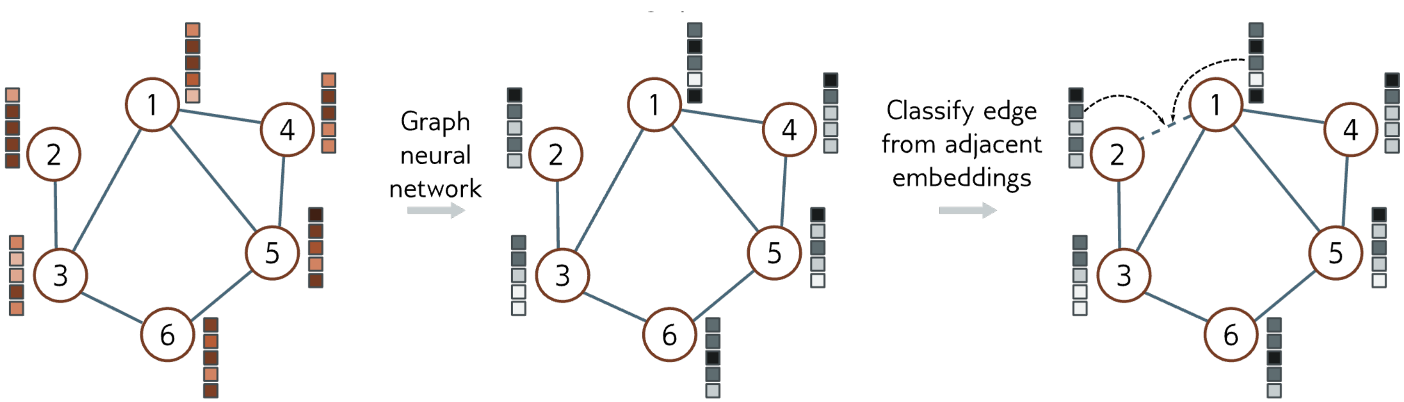


$$\Pr\left(y^{(n)} = 1 \middle| \mathbf{X}, \mathbf{A}\right) = \mathrm{sigmoid}[\beta_K + \omega_K \mathbf{h}_K^{(n)}]$$

$\mathbf{h}_K^{(n)}$ is the output embedding vector node for n

Edge prediction

Predict whether edge should exist or not.



$$\Pr\left(y^{(mn)} = 1 \middle| \mathbf{X}, \mathbf{A}\right) = \mathrm{sigmoid}[\mathbf{h}_K^{(m)T} \mathbf{h}_K^{(n)}]$$

Topics

- Basic definition and examples
- Graph representation
- Properties of Adjacency Matrix
- Graph neural network, tasks and loss functions
- Graph convolutional network
- Graph & Node classification
- Edge graphs

Graph convolutional network

These models are convolutional in that they update each node by aggregating information from nearby nodes.

As such, they induce a relational inductive bias (i.e., a bias toward prioritizing information from neighbors).

$$
\begin{aligned}
\mathbf{H}_1 &= \mathbf{F}[\mathbf{X}, \mathbf{A}, \phi_0] \\
\mathbf{H}_2 &= \mathbf{F}[\mathbf{H}_1, \mathbf{A}, \phi_1] \\
\mathbf{H}_3 &= \mathbf{F}[\mathbf{H}_2, \mathbf{A}, \phi_2] \\
\vdots &= \vdots \\
\mathbf{H}_K &= \mathbf{F}[\mathbf{H}_{K-1}, \mathbf{A}, \phi_{K-1}],
\end{aligned}
$$

A function $F[\cdot]$ with parameters ϕ_i that takes the node embeddings and adjacency matrix and outputs new node embeddings

Equivariance and Invariance

Every layer should be *equivariant* to index permutations

$$\mathbf{H}_{k+1}\mathbf{P} = \mathbf{F}[\mathbf{H}_k\mathbf{P}, \mathbf{P}^T\mathbf{A}\mathbf{P}, \phi_k]$$

And for node classification and edge prediction the output should be *invariant* to index permutations

$$y = \mathrm{sigmoid}[\beta_K + \omega_K \mathbf{H}_K \mathbf{1}/N\ ] = \mathrm{sigmoid}[\beta_K + \omega_K \mathbf{H}_K \mathbf{P}\mathbf{1}/N\ ]$$

Example Graph Convolution Network (GCN) layer

Aggregate information from neighboring nodes

$$\mathrm{agg}[n,k] = \sum_{m \in \mathrm{ne}[n]} \mathbf{h}_k^{(m)}$$

where $\mathrm{ne}[n]$ returns the set of indices of the neighbors of node n.

Example Graph Convolution Network (GCN) layer

Aggregate information from neighboring nodes

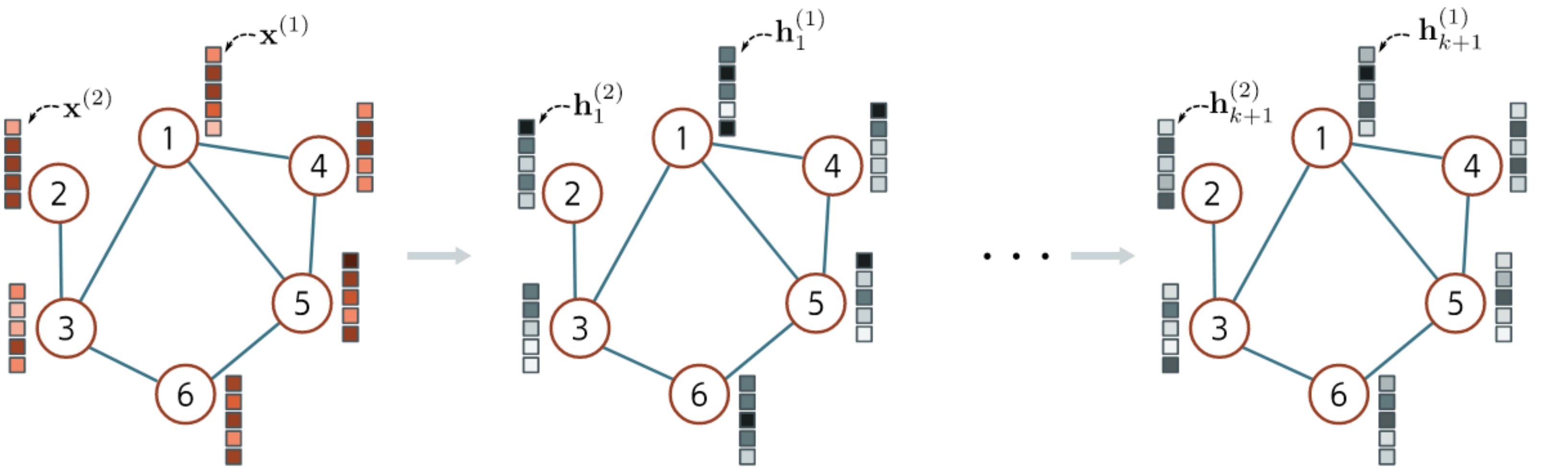
$$\mathrm{agg}[n,k] = \sum_{m \in \mathrm{ne}[n]} \mathbf{h}_k^{(m)}$$

where $\mathrm{ne}[n]$ returns the set of indices of the neighbors of node n.

Then a linear transform to the current node vector and the aggregate for the current node and add a bias.

$$\mathbf{h}_{k+1}^{(n)} = \mathbf{a}\left[\beta_k + \Omega_k \cdot \mathbf{h}_k^{(n)} + \Omega_k \cdot \mathrm{agg}[n,k]\right]$$

Graph convolution layers



$$\mathbf{h}_1^{(n)} = \mathbf{a}\left[\boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_1^{(n)} + \boldsymbol{\Omega}_0 \mathbf{agg}[n]\right]$$

$$\mathbf{h}_{k+1}^{(n)} = \mathbf{a}\left[\boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{h}_k^{(n)} + \boldsymbol{\Omega}_k \mathbf{agg}[n]\right]$$

Input

1st Layer

k+1st Layer

Example Graph Convolution Network (GCN) layer

We apply the following equation

$$\mathbf{h}_{k+1}^{(n)} = \mathbf{a}\left[\beta_k + \Omega_k \cdot \mathbf{h}_k^{(n)} + \Omega_k \cdot \mathrm{agg}[n,k]\right]$$

to the entire node hidden layers matrix, $\mathbf{H}_k$, by noting that $\mathbf{H}_k\mathbf{A}$ produces a matrix where the n^{th} column is $\mathrm{agg}[n,k]$.

$$\begin{aligned}\mathbf{H}_{k+1} &= \mathbf{a}\left[\boldsymbol{\beta}_k\mathbf{1}^T + \boldsymbol{\Omega}_k\mathbf{H}_k + \boldsymbol{\Omega}_k\mathbf{H}_k\mathbf{A}\right] \\ &= \mathbf{a}\left[\boldsymbol{\beta}_k\mathbf{1}^T + \boldsymbol{\Omega}_k\mathbf{H}_k(\mathbf{A}+\mathbf{I})\right],\end{aligned}$$

Example Graph Convolution Network (GCN) layer

We apply the following equation

$$\mathbf{h}_{k+1}^{(n)} = \mathbf{a}\left[\beta_k + \Omega_k \cdot \mathbf{h}_k^{(n)} + \Omega_k \cdot \text{agg}[n,k]\right]$$

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Note that this is (1) equivariant to permutations, (2) handles arbitrary number of neighbors, (3) exploits graph structure and (4) share parameters

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Graph classification example

We can put it all together and add a sigmoid layer

$$
\begin{aligned}
\mathbf{H}_1 &= \mathbf{a}\left[\boldsymbol{\beta}_0\mathbf{1}^T + \boldsymbol{\Omega}_0\mathbf{X}(\mathbf{A}+\mathbf{I})\right] \\
\mathbf{H}_2 &= \mathbf{a}\left[\boldsymbol{\beta}_1\mathbf{1}^T + \boldsymbol{\Omega}_1\mathbf{H}_1(\mathbf{A}+\mathbf{I})\right] \\
\vdots &= \vdots \\
\mathbf{H}_K &= \mathbf{a}\left[\boldsymbol{\beta}_{K-1}\mathbf{1}^T + \boldsymbol{\Omega}_{K-1}\mathbf{H}_{k-1}(\mathbf{A}+\mathbf{I})\right] \\
\mathrm{f}[\mathbf{X},\mathbf{A},\boldsymbol{\Phi}] &= \mathrm{sig}\left[\beta_K + \boldsymbol{\omega}_K\mathbf{H}_K\underbrace{\mathbf{1}/N}_{\text{Mean pooling}}\right],
\end{aligned}
$$

For classification on molecules,

$X \in \mathbb{R}^{118\times N}$: one hot encoding of 118 elements

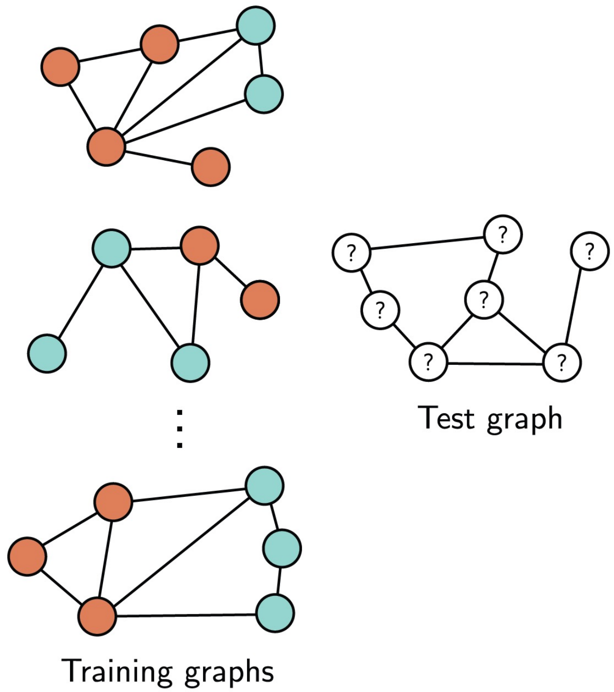
$\Omega_0 \in \mathbb{R}^{D\times 118}$: convert to D-dimensional embeddings

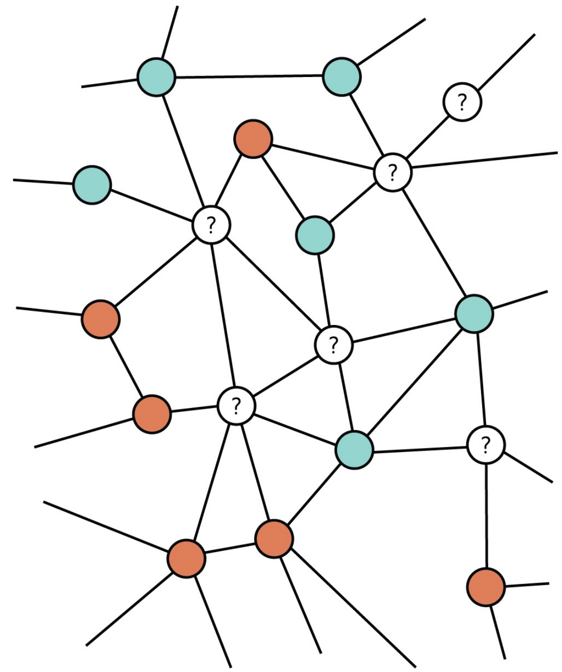
β_K: is a scalar

ω_K: a $1\times D$ parameters row vector

You'll be implementing this in notebook 13.2.

Inductive vs. Transductive





supervised learning: train with the labeled graphs and then run inference on the unlabeled (test) graphs

semi-supervised learning: train with the labeled nodes, then run inference to determine label for unlabeled nodes

Node classification example

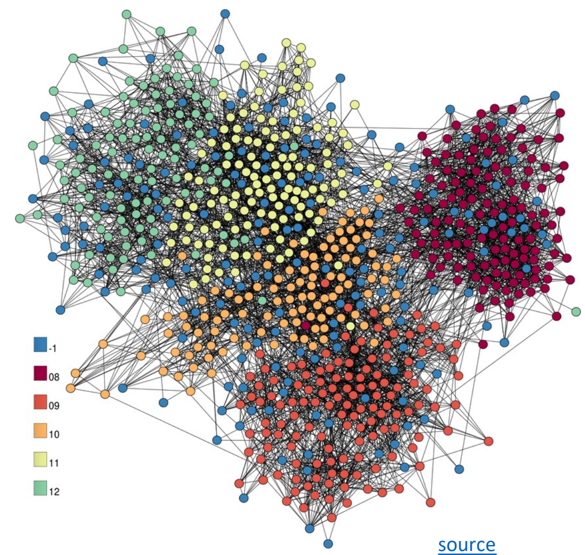
Assume *transductive* binary node *classification* with millions of nodes, *partially labeled*.

Same network body as graph classification, but different head:

$$\mathbf{f}[\mathbf{X}, \mathbf{A}, \boldsymbol{\Phi}] = \text{sigmoid}[\beta_K \mathbf{1}^T + \boldsymbol{\omega}_K \mathbf{H}_K]$$

No mean pooling. Output is $1 \times N$.

Train with binary cross-entropy loss on nodes with labels.



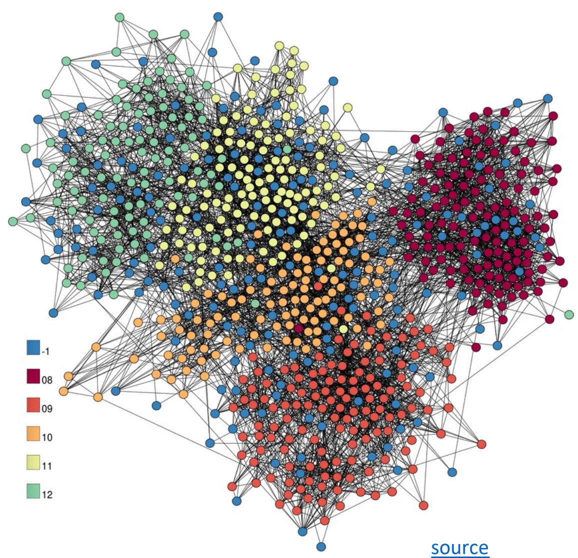
source

Node classification example

Assume *transductive* binary node *classification* with <u>millions of nodes</u>, *partially labeled*.

Challenges:

1. memory limitations: need to store every node and hidden layer embedding during training
2. how to perform SGD with basically one batch!



source

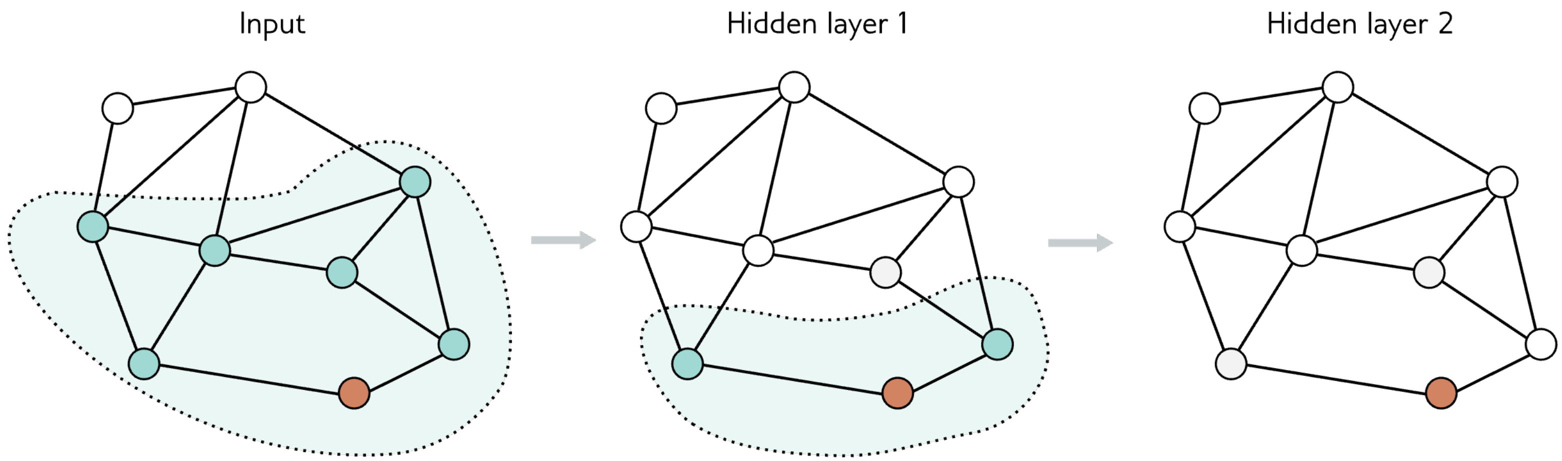
Solutions: Choosing batches for graphs

1. Choose random subset of nodes

2. Neighborhood sampling

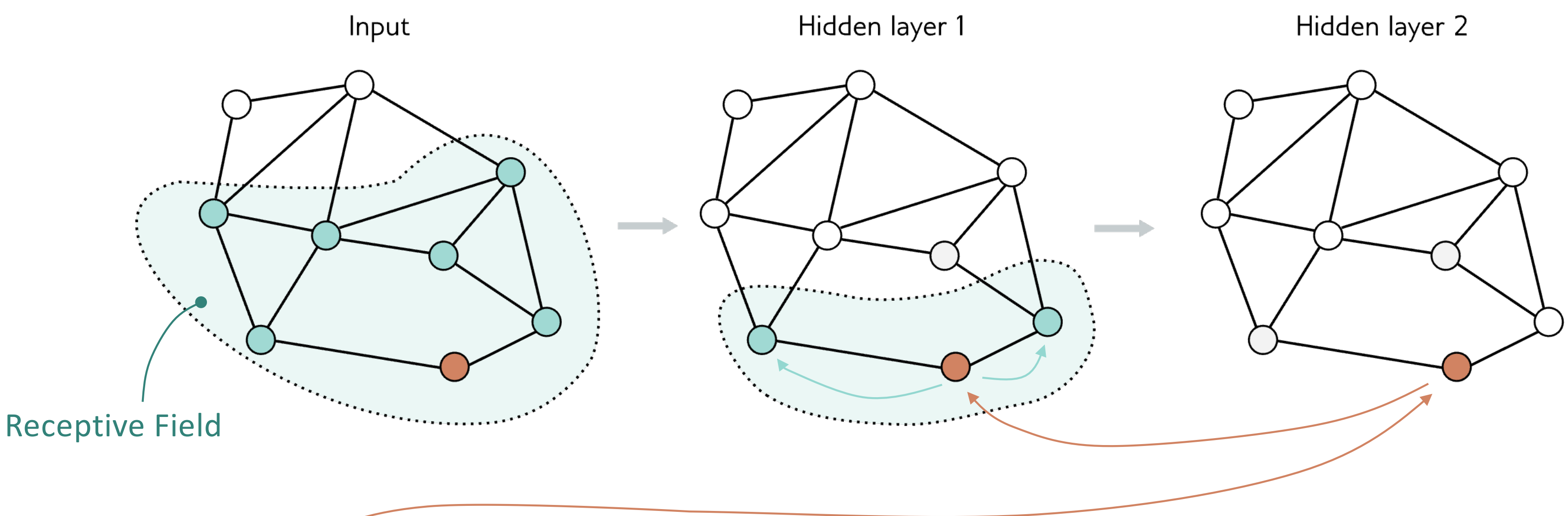
3. Graph partitioning

Batches: Random subset



You can pick a random batch of labeled nodes at each training step.

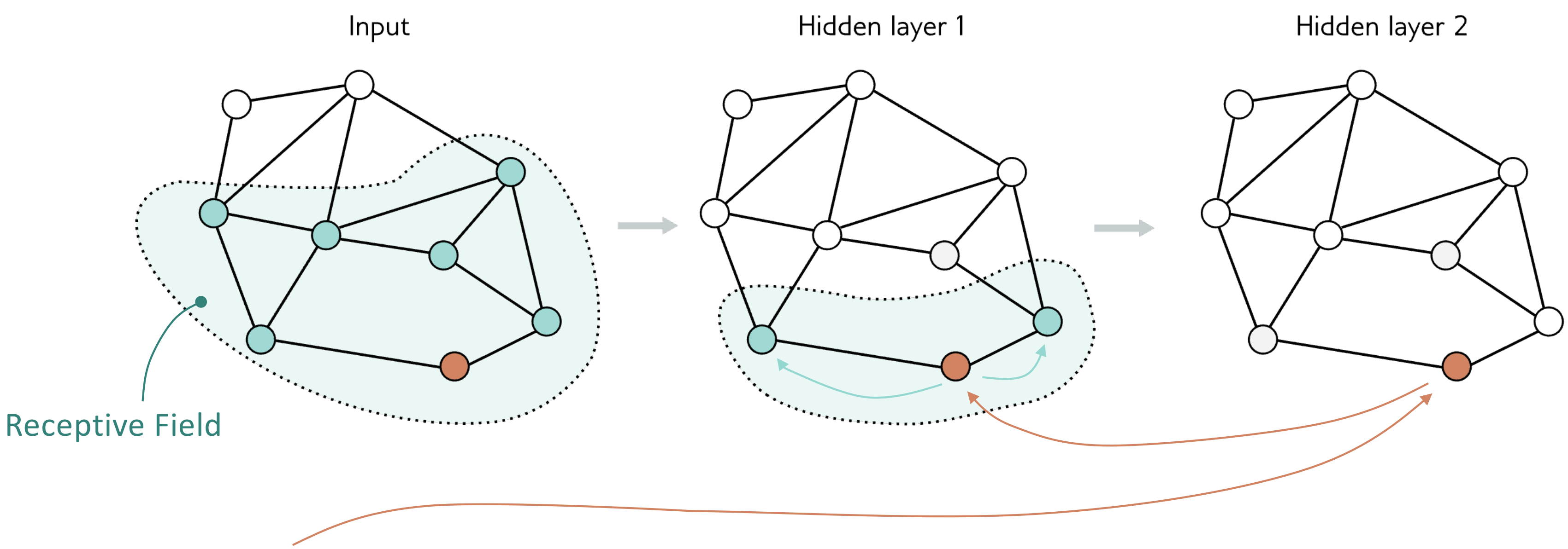
Batches: Random subset



Each node is dependent on the same node in the previous layer and its neighbors because of agg[]

$$\mathbf{h}_{k+1}^{(n)} = \mathbf{a}\left[\beta_k + \Omega_k \cdot \mathbf{h}_k^{(n)} + \Omega_k \cdot \text{agg}[n,k]\right]$$

Batches: Random subset

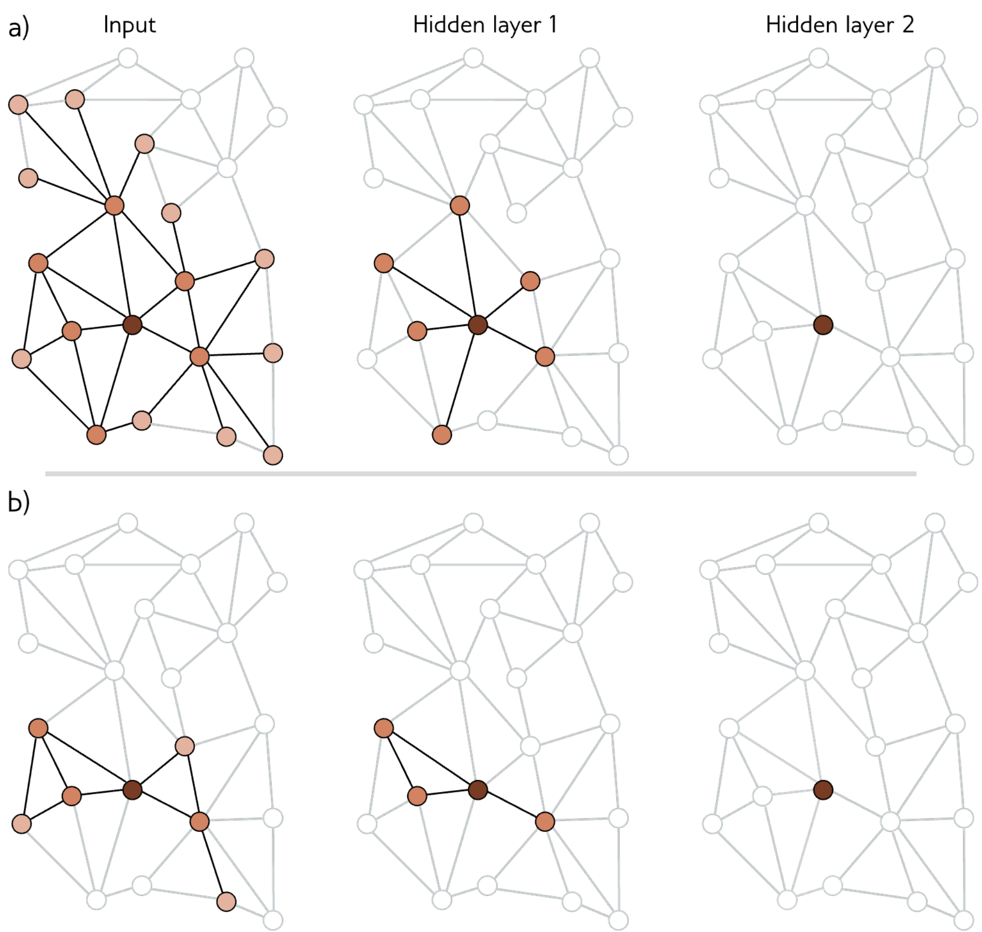


Each node is dependent on the same node in the previous layer and its neighbors because of agg[].

$$\mathbf{h}_{k+1}^{(n)} = \mathbf{a}\left[\beta_k + \Omega_k \cdot \mathbf{h}_k^{(n)} + \Omega_k \cdot \mathrm{agg}[n,k]\right]$$

With many layers and dense connection, it can quickly expand to encompass every node.

Neighborhood Sampling



Random Sampling:

Use all the neighbors

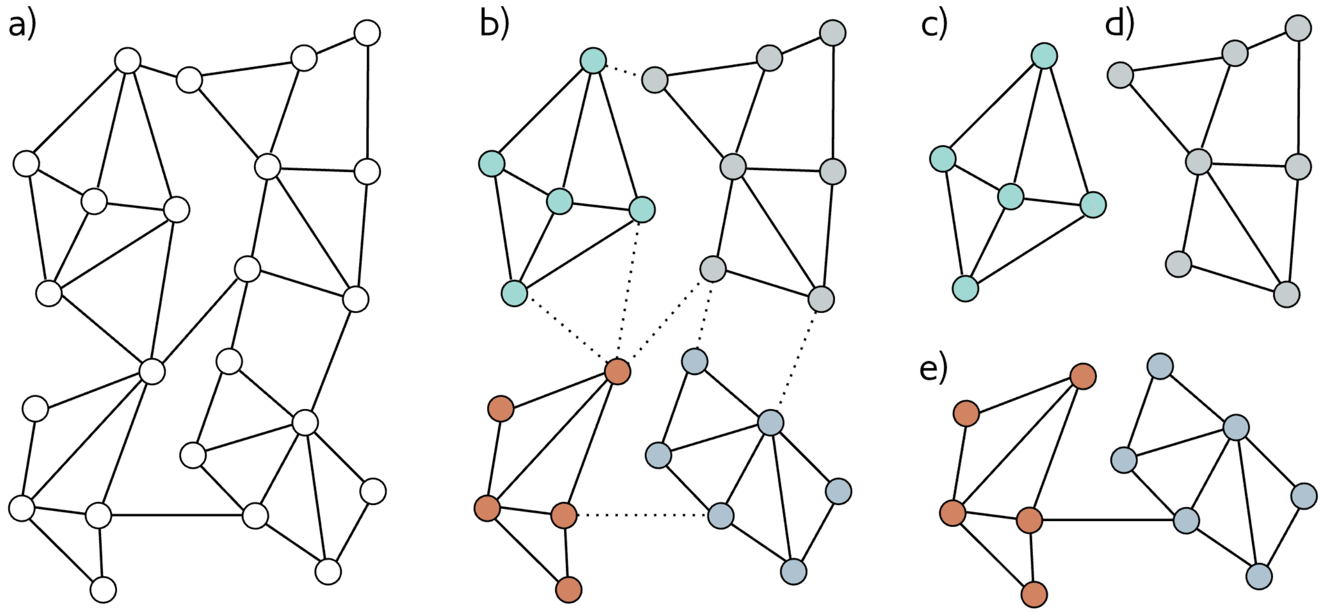
Neighborhood Sampling:

Use max n of the neighbors.

Here $n = 3$.

Notebook 13.3

Graph Partitioning



Disconnect edges of the original to create maximally connected disjoint subsets

Split into train, test and validation sets and train just like in the inductive setting.

Alternatives to Mean Pooling for Node Combinations

- **Diagonal enhancement**: current node is multiplied by $(1+\epsilon_k)$, where ϵ_k is a learned scalar for each layer

$$\mathbf{H}_{k+1} = \mathbf{a}[\beta_k \mathbf{1}^T + \boldsymbol{\Omega}_k \mathbf{H}_k(\mathbf{A} + (1+\epsilon_k)\mathbf{I})]$$

- **Residual connections**: Include the current node in the sum

$$\mathbf{H}_{k+1} = \mathbf{a}[\beta_k \mathbf{1}^T + \boldsymbol{\Omega}_k \mathbf{H}_k \mathbf{A})] + \mathbf{H}_k$$

- **Mean aggregation**: take average instead of sum of neighbors

$$\mathrm{agg}[n] = \frac{1}{|\mathrm{ne}[n]|} \sum_{m \in \mathrm{ne}[n]} \mathbf{h}_m$$

- **Kipf normalization**: downweight neighboring nodes with a lot of neighbors

$$\mathrm{agg}[n] = \sum_{m \in \mathrm{ne}[n]} \frac{h_m}{\sqrt{|\mathrm{ne}[n]||\mathrm{ne}[m]|}}$$

- **Max pool aggregation**: element-wise max of all neighbors to current node

$$\mathrm{agg}[n] = \max_{m \in \mathrm{ne}[n]} [\mathbf{h}_m]$$

Aggregation by Attention

Weights depend on data at the nodes.

Apply linear transform to current node:

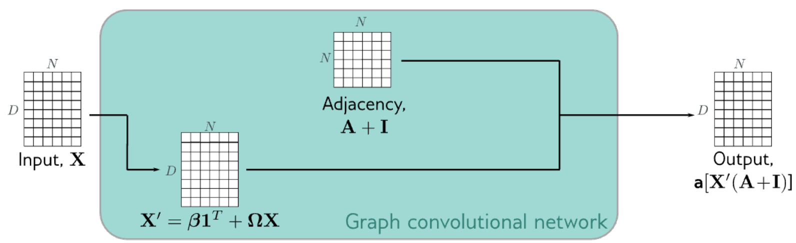
$$\mathbf{H'}_k = \beta_k \mathbf{1}^T + \mathbf{\Omega}_k \mathbf{H}$$

Then the similarity s_{mn} of each transformed node embedding $\mathbf{h'}_m$ to the transformed node embedding $\mathbf{h'}_n$ is computed by concatenating the pairs, taking a dot product with a column vector ϕ_k of learned parameters, and applying an activation function:

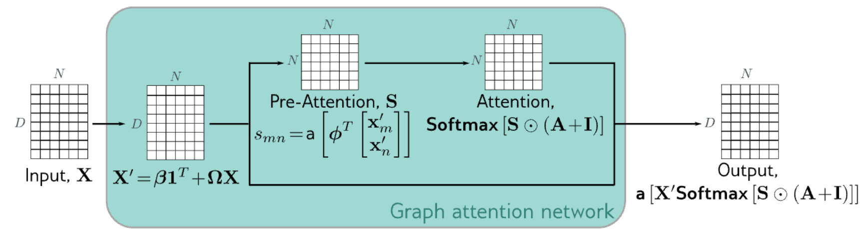
$$s_{mn} = \mathrm{a}\left[\phi_k^T \begin{bmatrix} \mathbf{h'}_m \\ \mathbf{h'}_n \end{bmatrix}\right]$$

$$\mathbf{H}_{k+1} = \mathbf{a}[\mathbf{H'}_k \cdot \mathrm{Softmask}[\mathbf{S}, \mathbf{A} + \mathbf{I}]]$$

Graph Attention

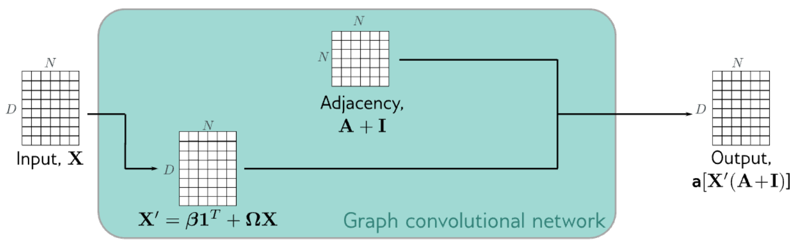


Regular graph convolution

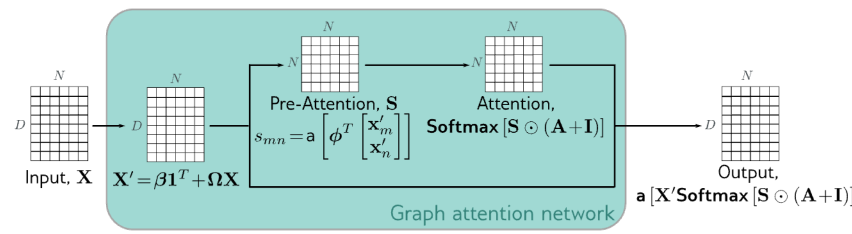


Graph attention

Graph Attention

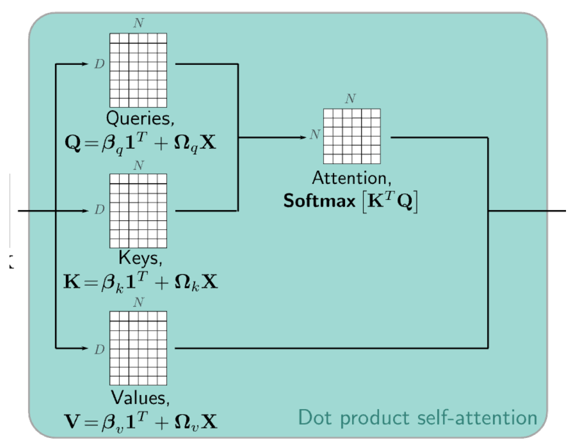


Regular graph convolution



Graph attention

Transformer se



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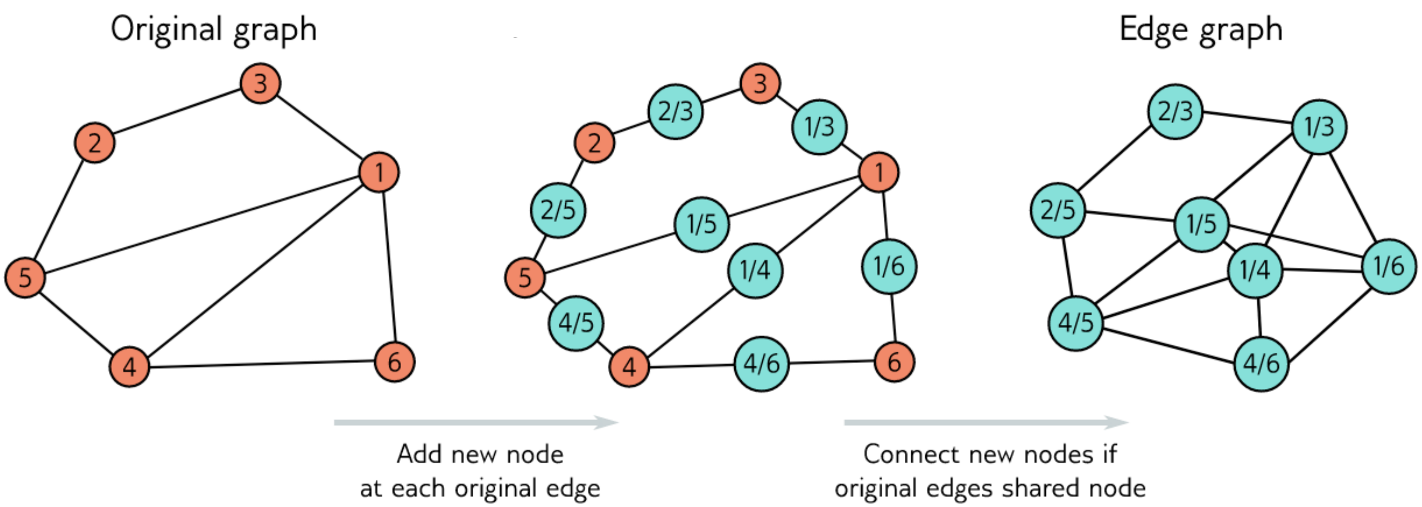
Edge Graphs



Handled by simple transformation from node graphs.

Next

- Reinforcement Learning
- Joint Embedding Predictive Architecture
- Project Presentations

Feedback?

Link