CSDS503 / COMP552 – Advanced Machine Learning

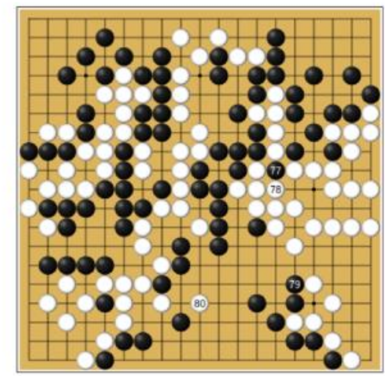
Faizad Ullah

Traditional Neural Networks

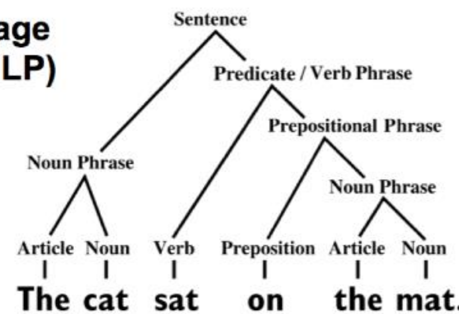
IMAGENET

Speech data

Grid games



Natural language processing (NLP)



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Deep neural nets that exploit:

- translation equivariance (weight sharing)
- hierarchical compositionality

* slide from Thomas Kipf, **University of Amsterdam**

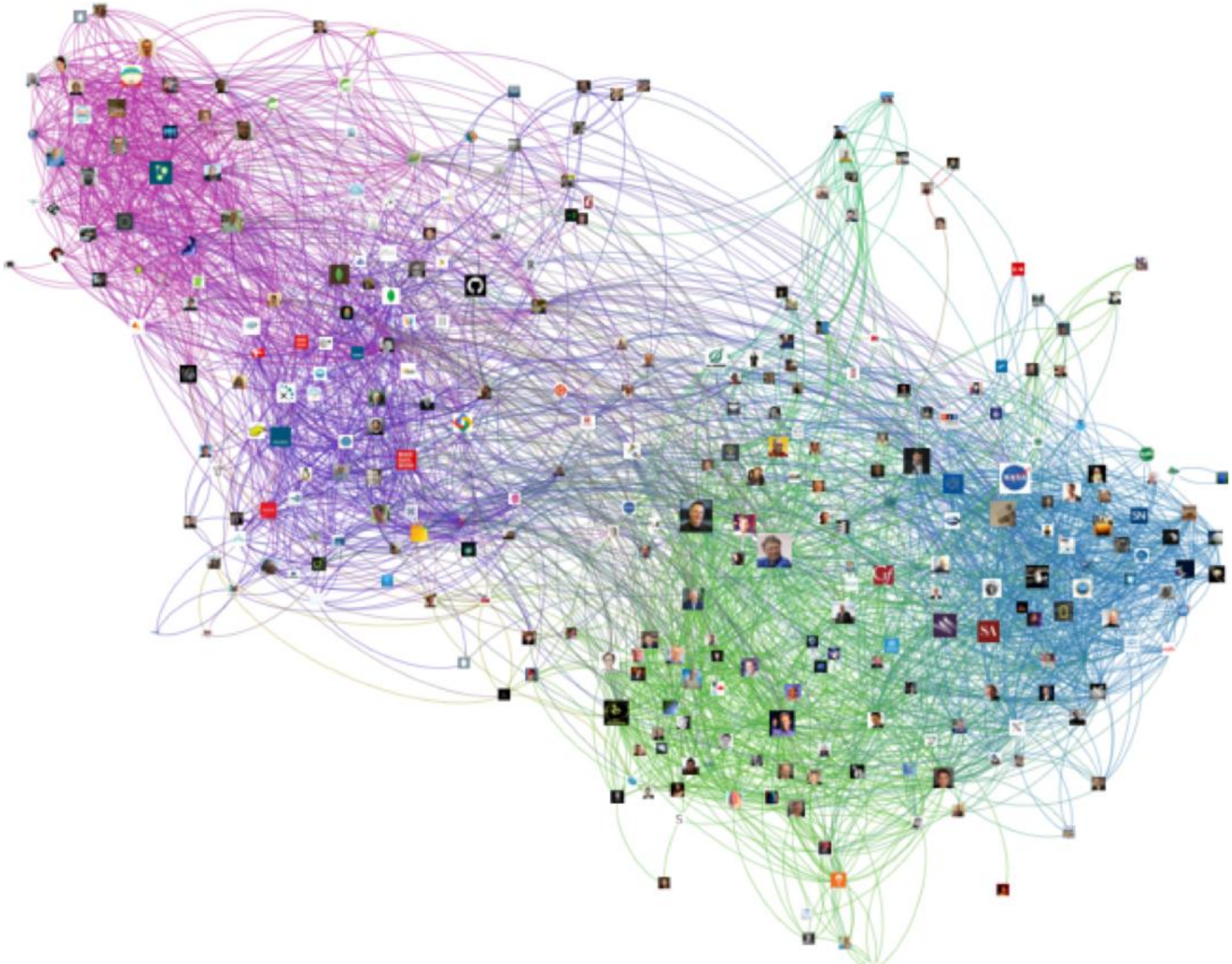
Graph-structured Data

- A lot of real-world data does not “live” on grids

Social Networks

Standard **CNN** and **RNN** architectures don’t work on this data

Twitter followers graph

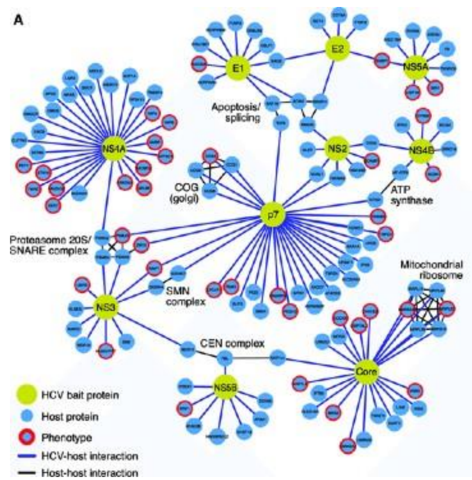


http://allthingsgraphed.com/2014/11/02/twitter-friends-network/

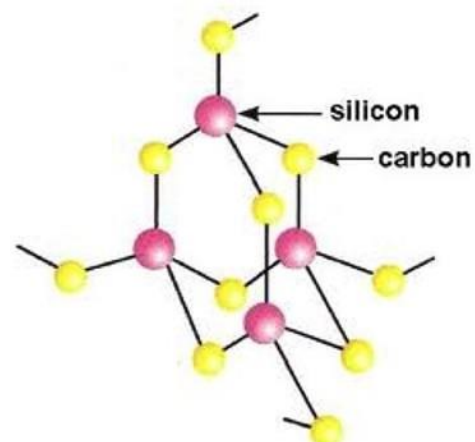
Graph-structured Data

- A lot of real-world data does not “live” on grids

Social Networks



Protein Networks

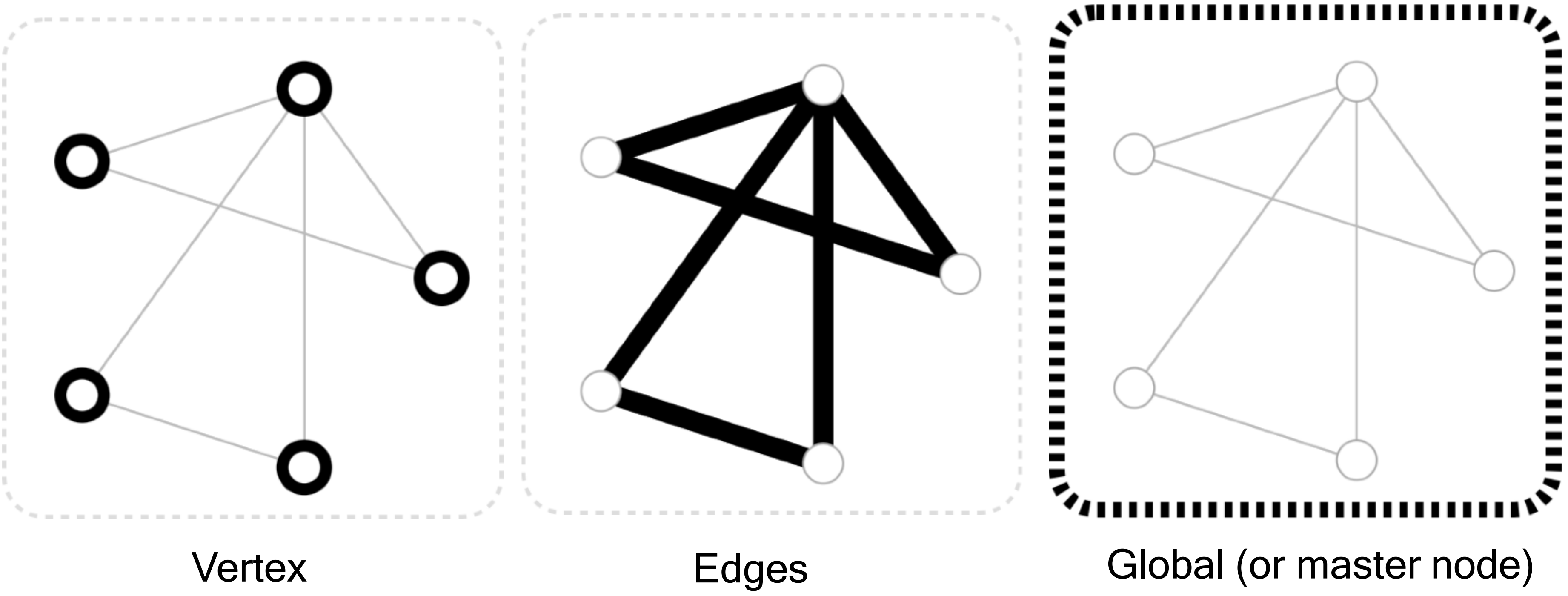


Molecules

Standard **CNN** and **RNN** architectures don’t work on this data

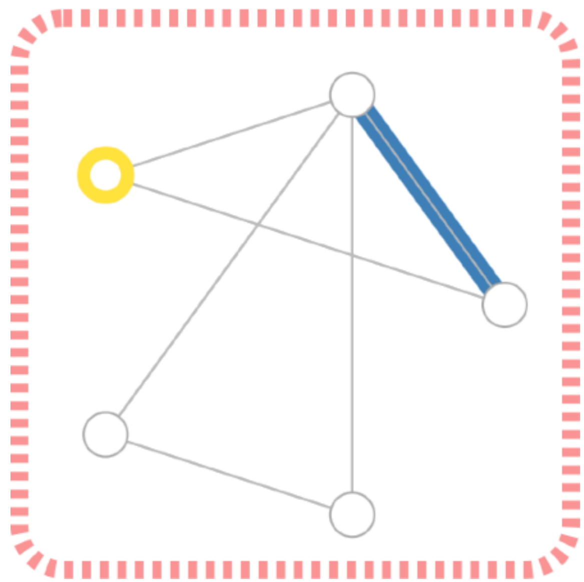
Graph

- A set of objects, and the connections between them, are naturally expressed as a *graph*.
- A graph represents the relations (*edges*) between a collection of entities (*nodes*).



Graph

A graph is a pair $G = (V, E)$, where $V = \{1, \cdots, n\}$is a set of *n* vertices (nodes), and $E = \{(i, j) \,|\, i, j \in N\}$ is a set of edges between them.



Graph

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- Alternatively, we can define an adjacency matrix A where:

$$A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$$

- If $A^T = A$, we say the graph is undirected.

Images as graphs

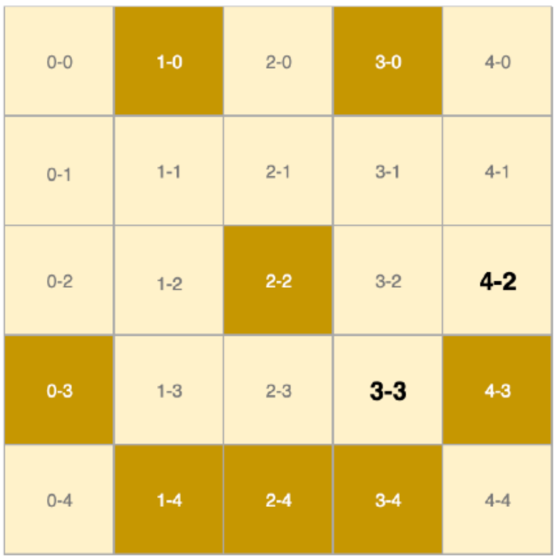
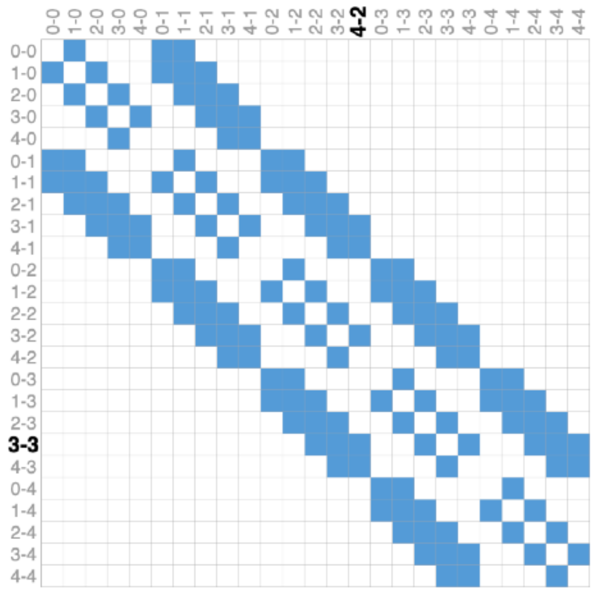
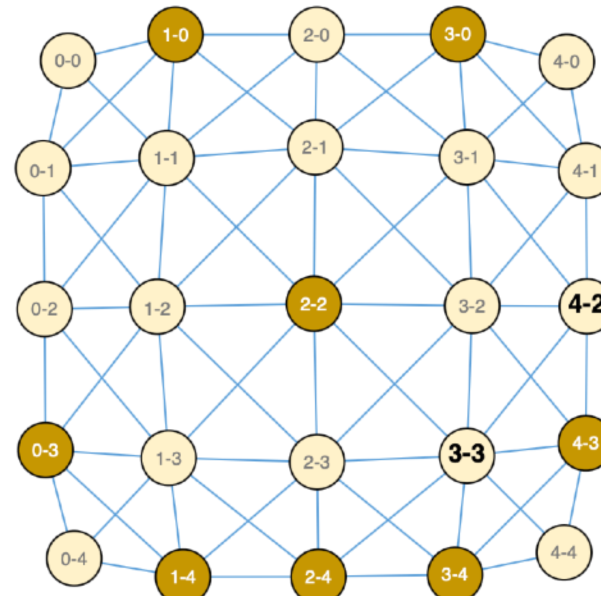


Image Pixels



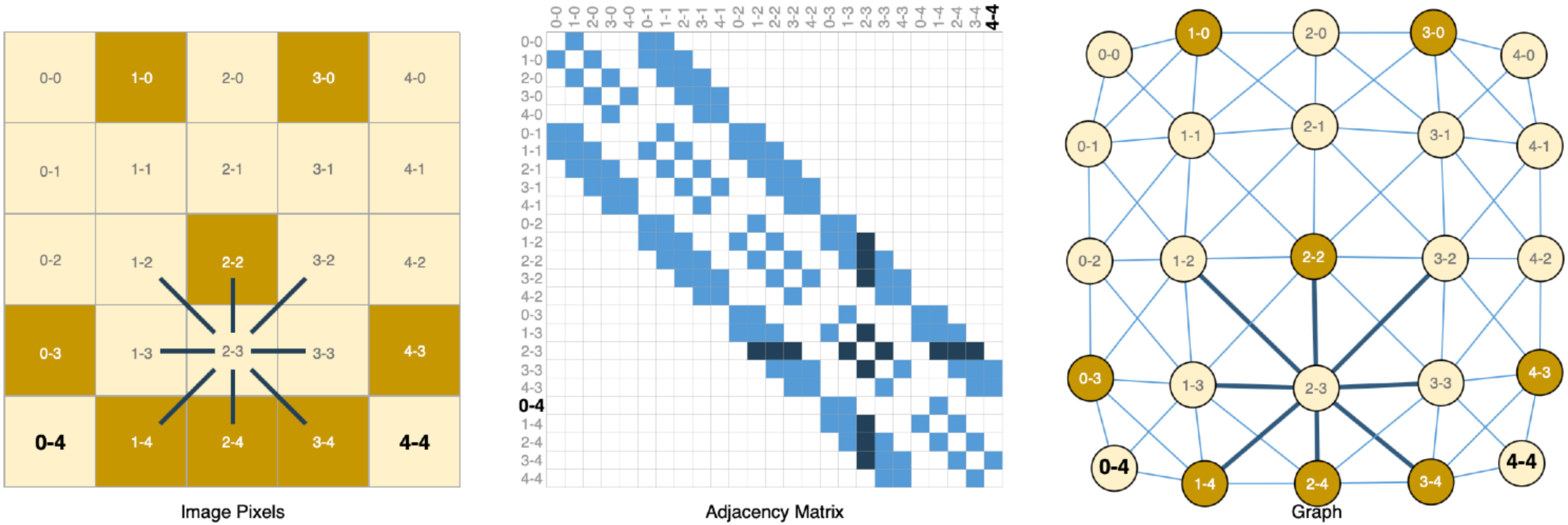
Adjacency Matrix



Graph

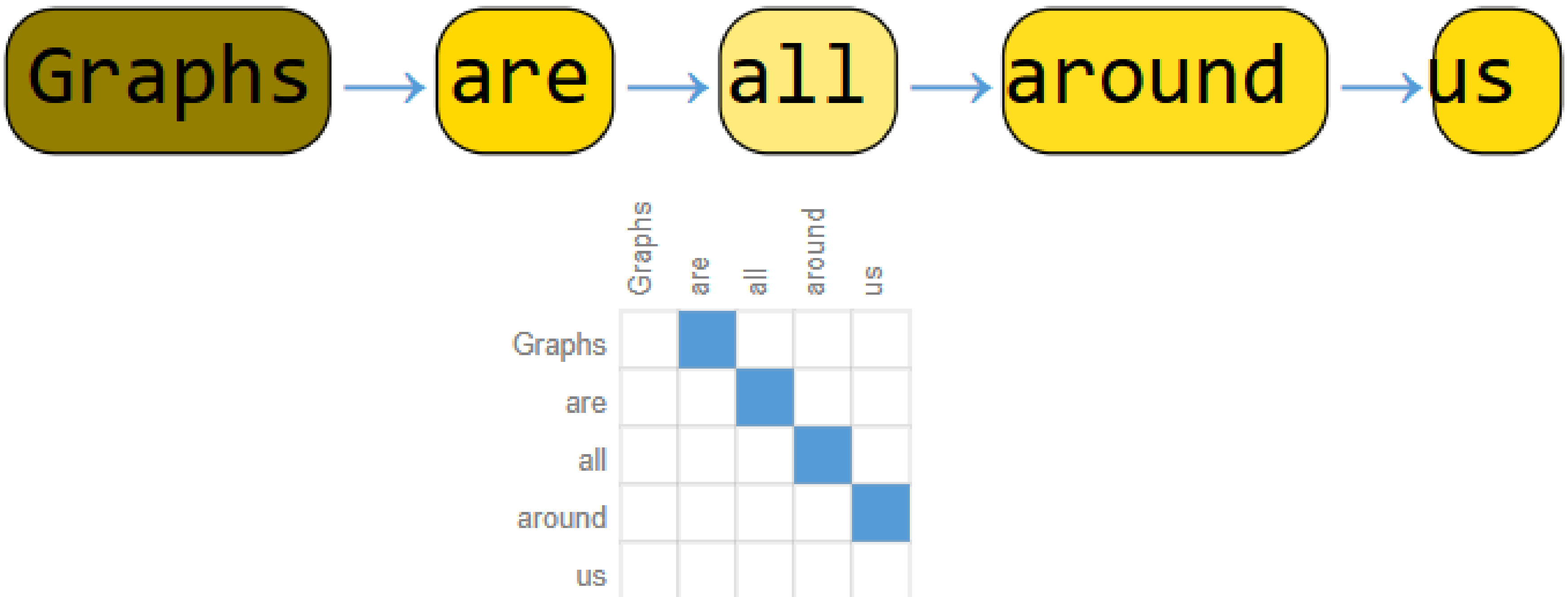
https://distill.pub/2021/gnn-intro/

Images as graphs

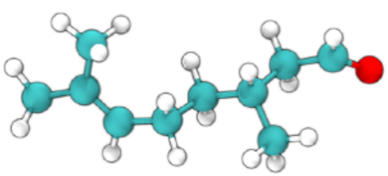


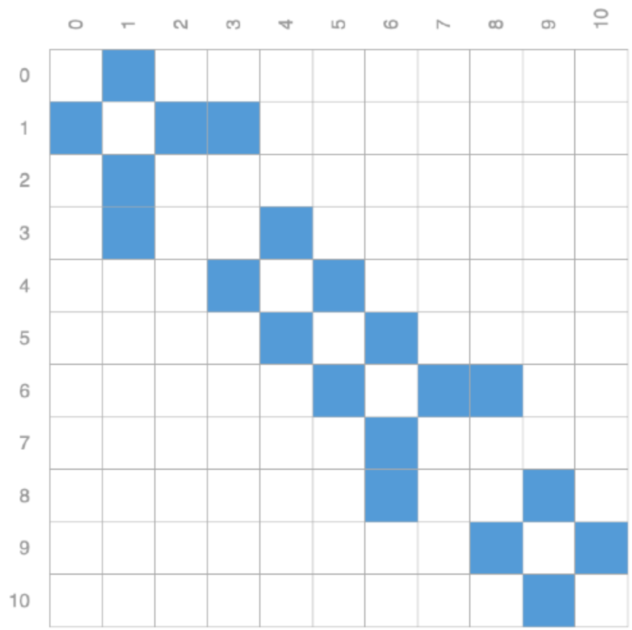
https://distill.pub/2021/gnn-intro/

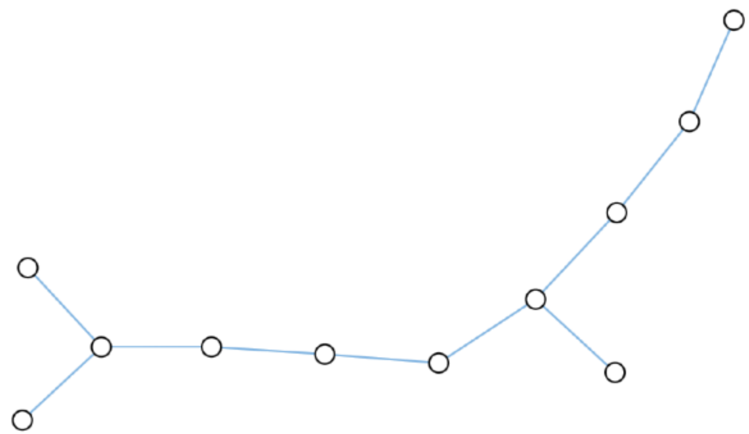
Text as graphs



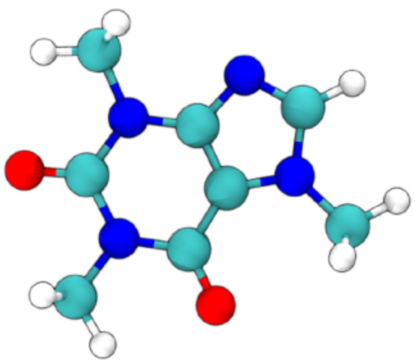
Molecules as graphs

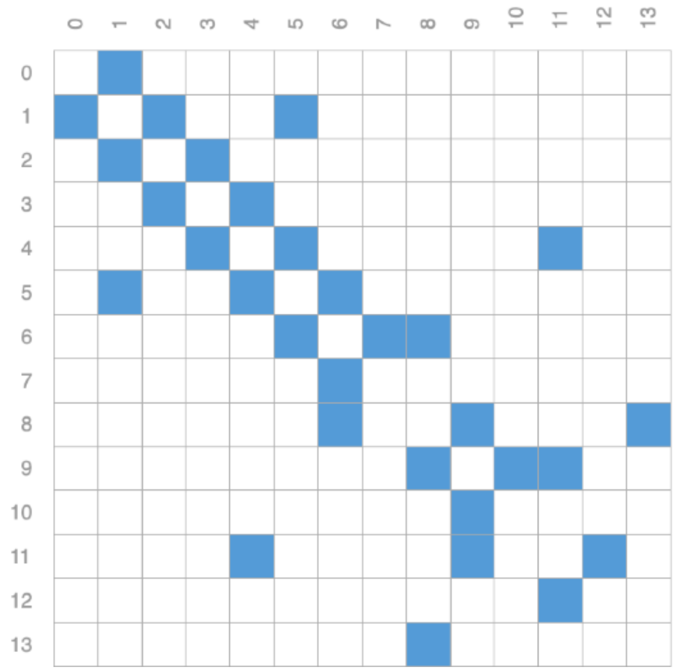


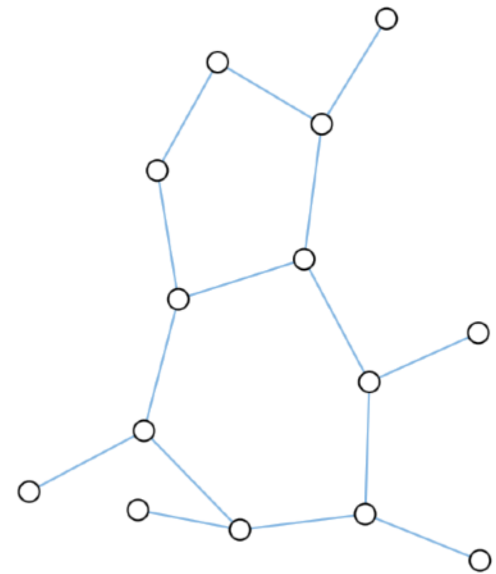




Molecules as graphs







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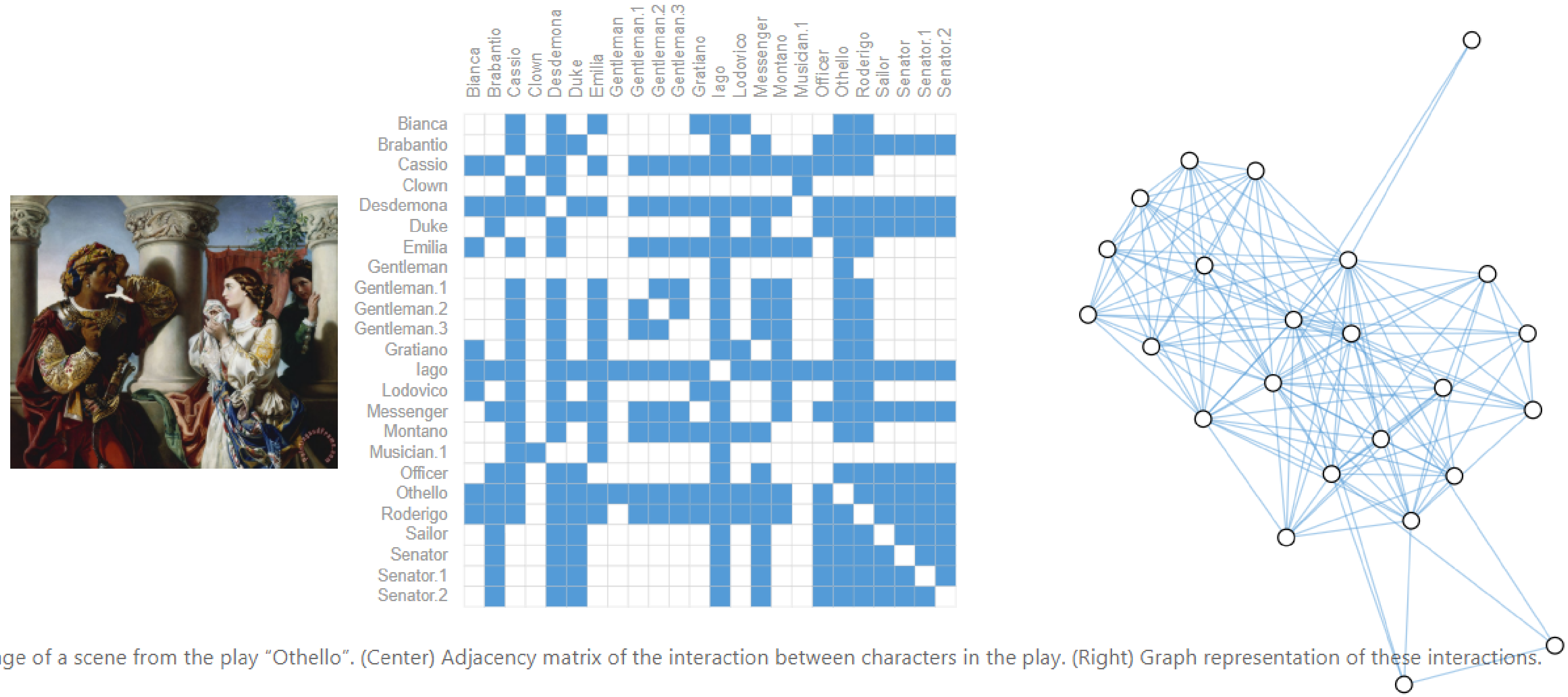
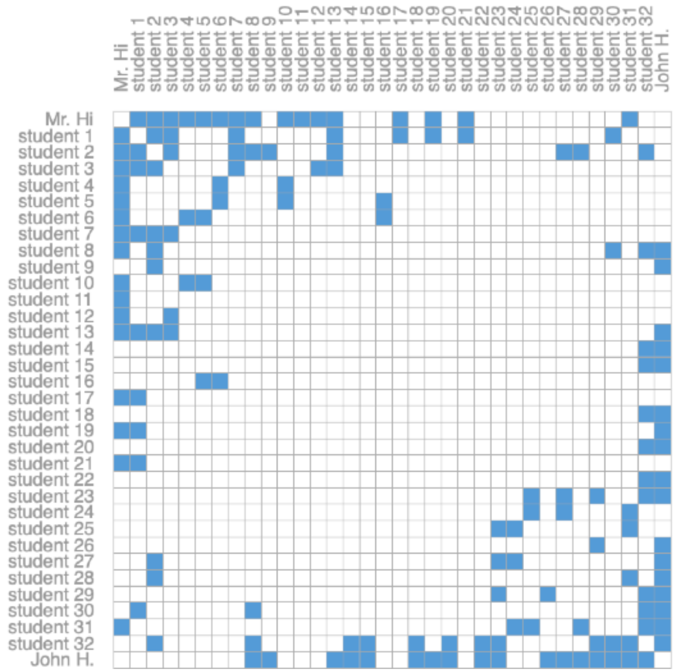
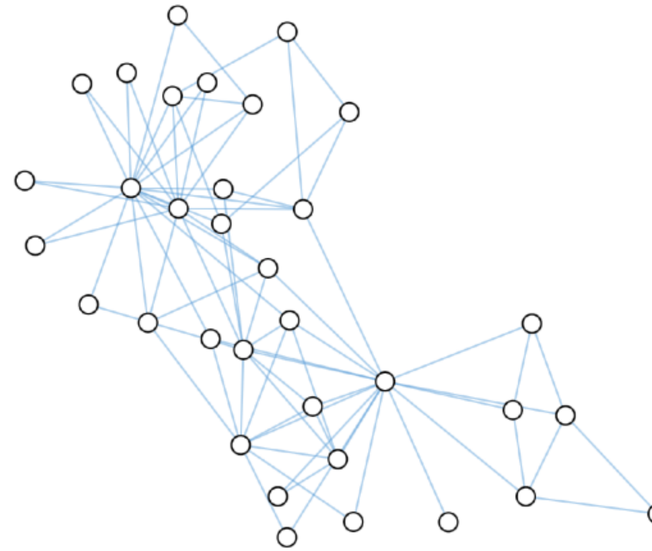
Social networks as graphs



(Left) Image of a scene from the play “Othello”. (Center) Adjacency matrix of the interaction between characters in the play. (Right) Graph representation of these interactions.

Social Network as Graph





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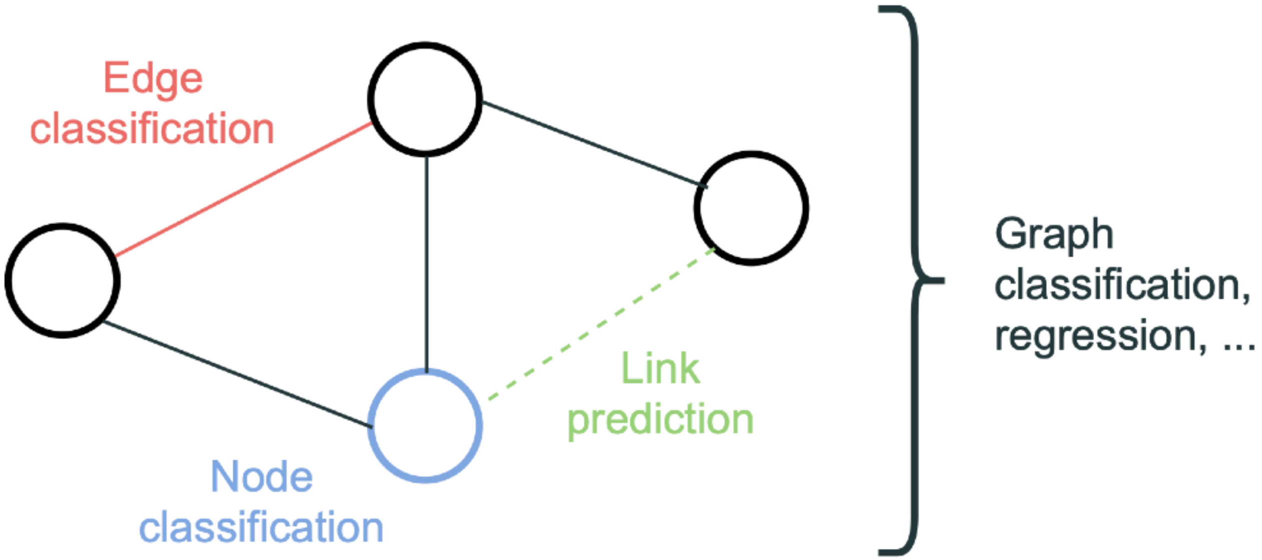
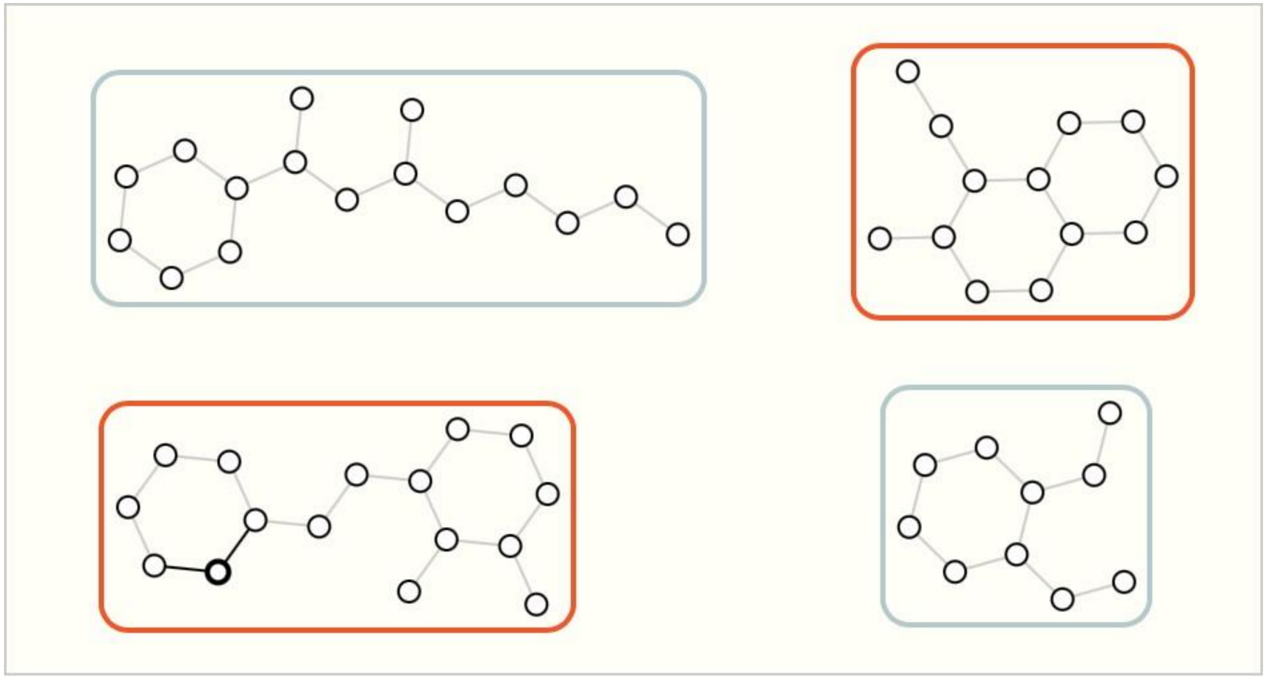
Learning Problems on Graphs

Learning Problems on Graphs



https://www.sscardapane.it/assets/files/nnds2021/Lecture_6_graphs.pdf

Graph-level task

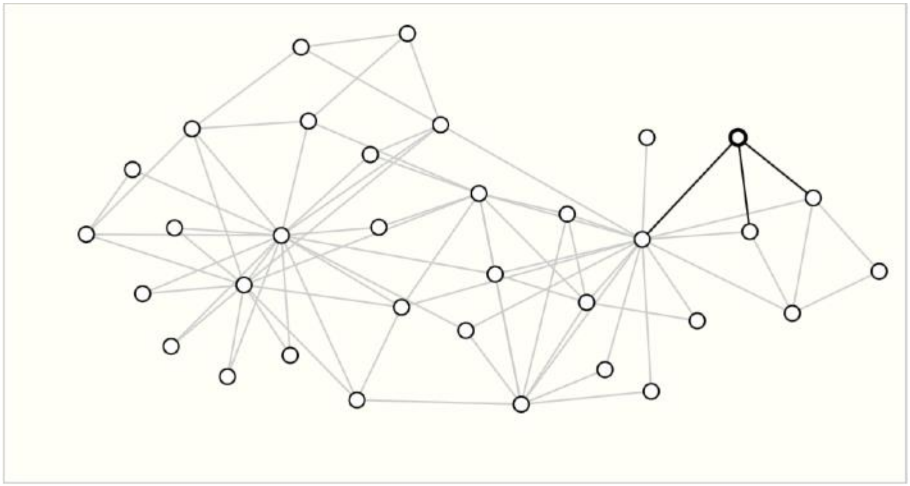


Output: labels for each graph, (e.g., "does the graph contain two rings?")

This is analogous to image classification problems with MNIST and CIFAR, where we want to associate a label to an entire image. With text, a similar problem is sentiment analysis where we want to identify the mood or emotion of an entire sentence at once.

Node-level task

- Node-level tasks are concerned with predicting the identity or role of each node within a graph.
- The prediction problem is to classify whether a given member becomes loyal to either Mr. Hi or John H.



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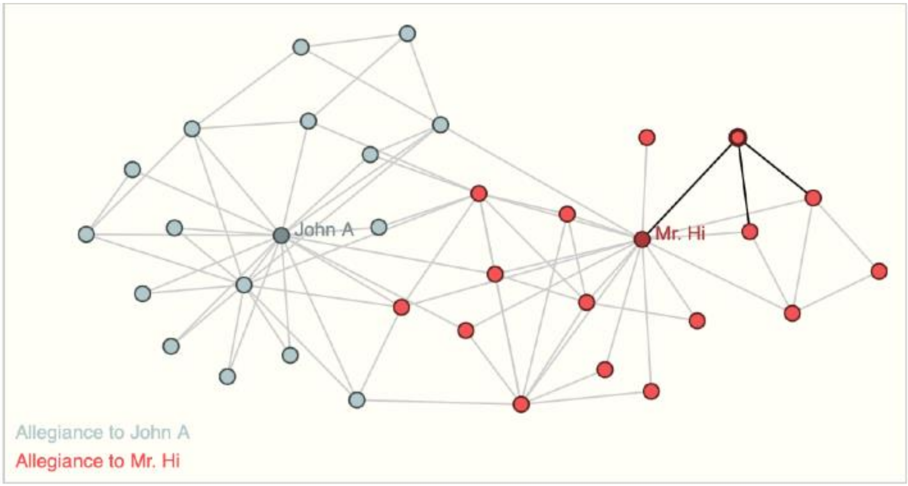
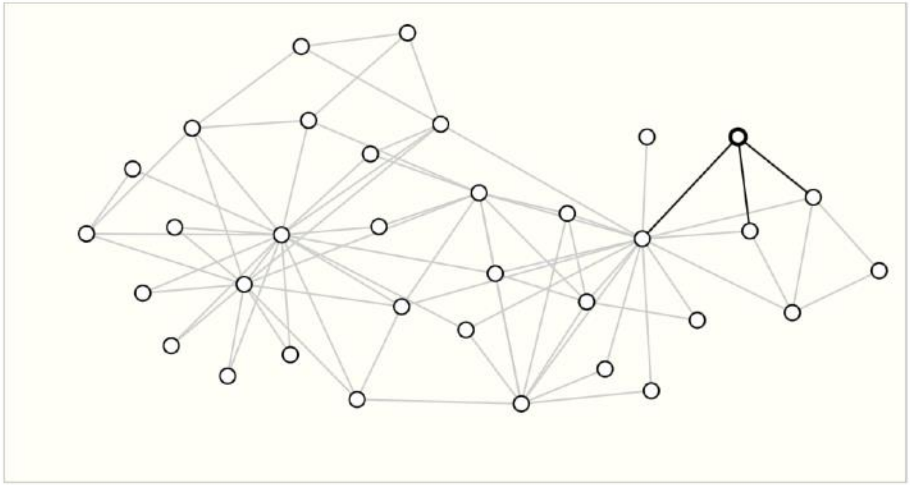


Input: graph with unlabled nodes

Output: graph node labels



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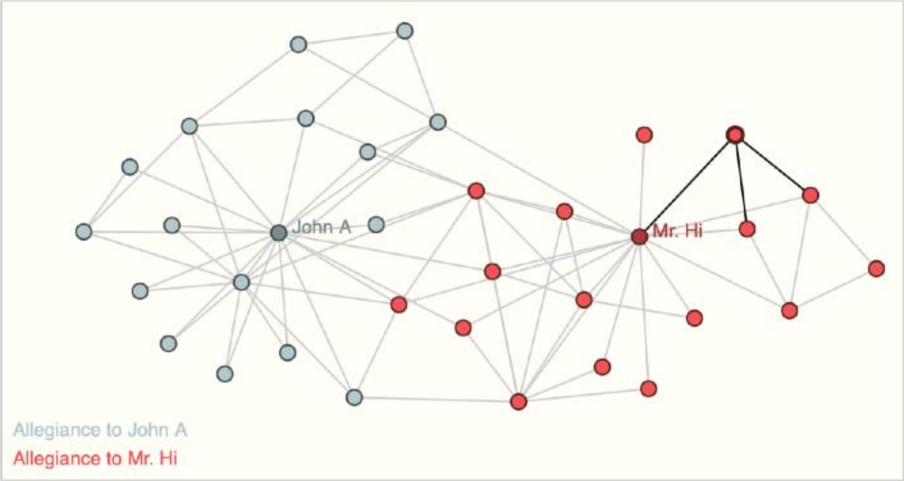
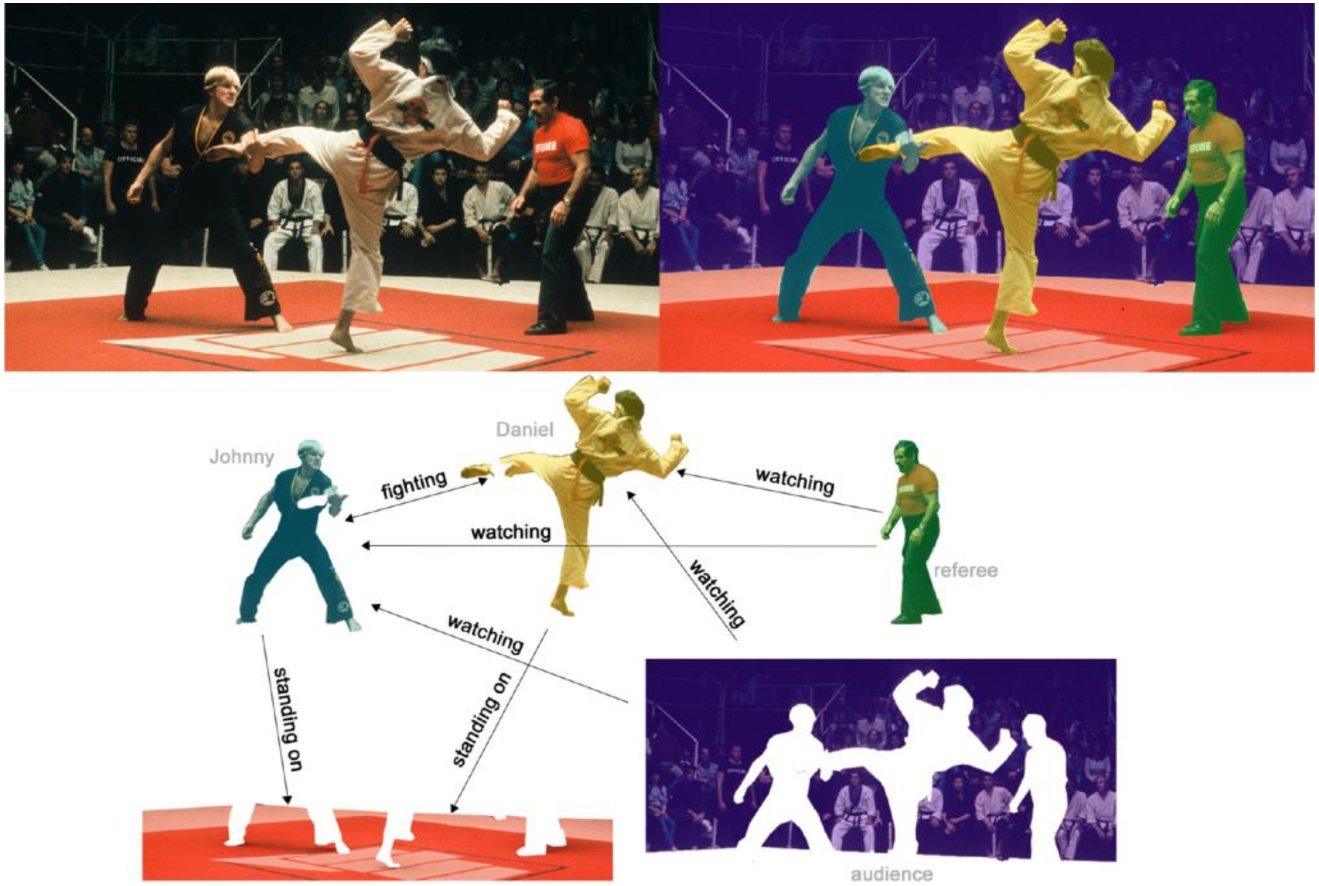


Input: graph with unlabled nodes

Output: graph node labels

Edge-level task

- Beyond identifying objects in an image, deep learning models can be used to predict the relationship between them.



https://distill.pub/2021/gnn-intro/

Edge-level task

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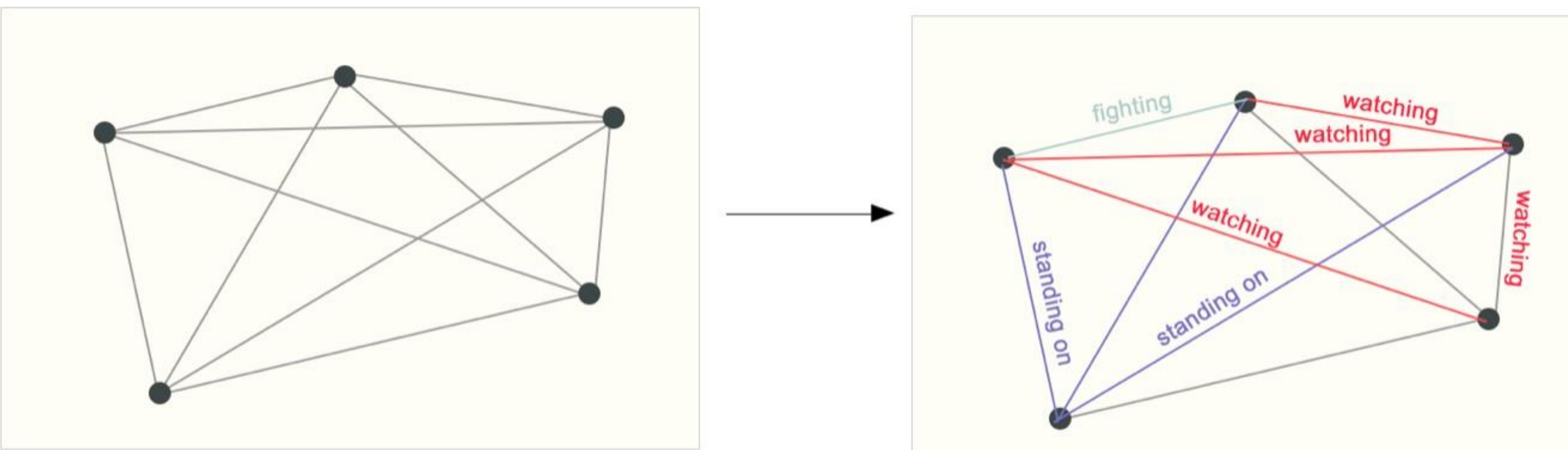

Input: fully connected graph, unlabeled edges **Output:** labels for edges

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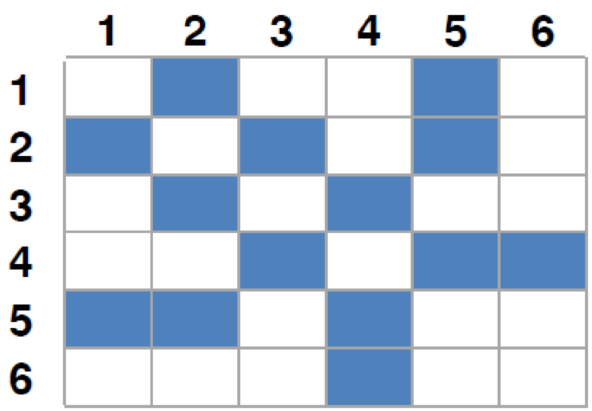
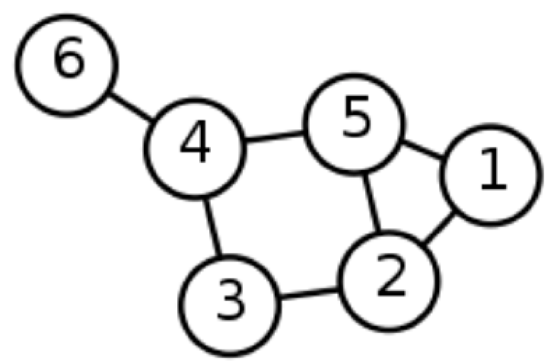
Graph: Neighbours and degrees

- The neighborhood $\mathcal{N}_i$ of a node i is defined as the set of nodes sharing an edge with the node:

$$\mathcal{N}_i = \{j \,|\, A_{ij} = 1\}\,.$$



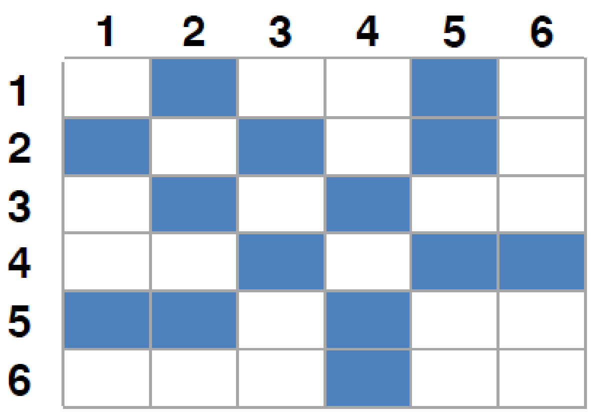


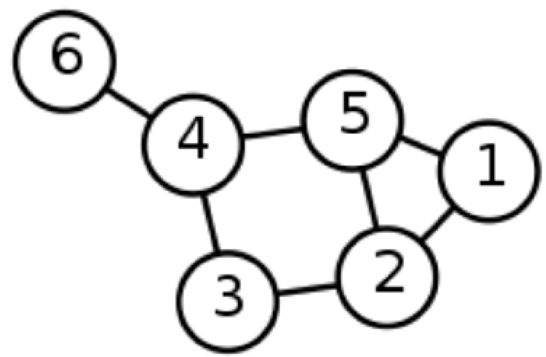
$$\mathcal{N}_4 = \{3,\, 5,\, 6\}\,.$$

Graph: Neighbours and degrees

- The size $|\mathcal{N}_i|$ of the neighborhood is called the degree of the node. The degree matrix D is a diagonal matrix containing the degrees:

$$[D]_{i,i} = \sum_j A_{ij}\,.$$

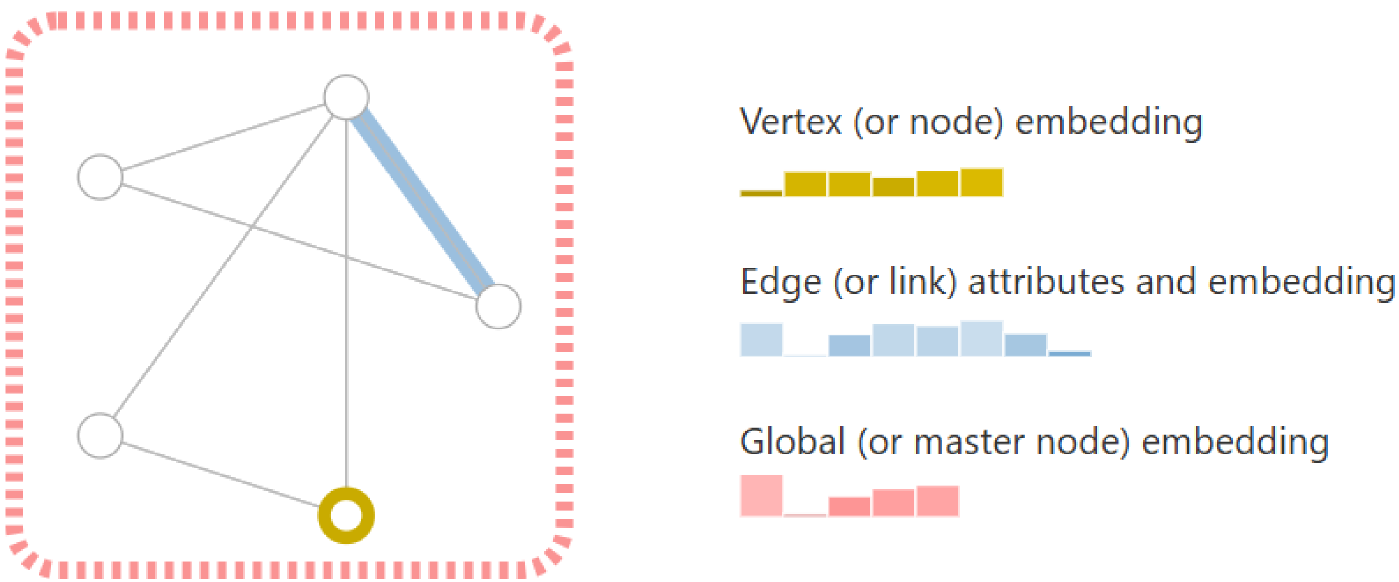




$$[D]_{4,4} = \sum_j A_{4j} = 3$$

Features on a graph

- Depending on the application, we can have node features x_i, edge features $\mathbf{e}_{ij}$, or graph features.



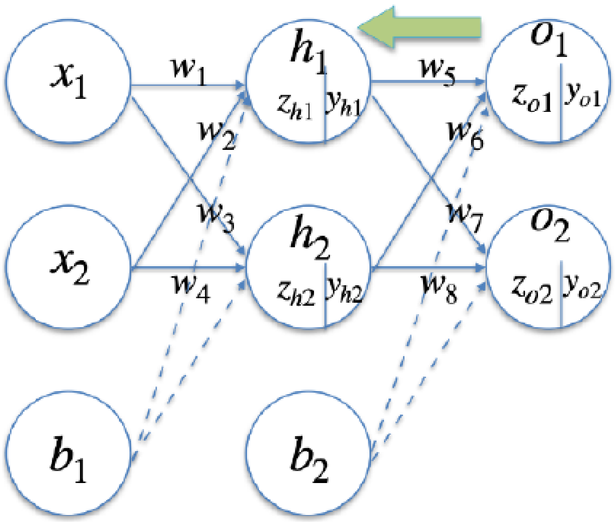
Information in the form of scalars or embeddings can be stored at each graph node (left) or edge (right).

- In the simplest case, we associate to each node a vector$_i$ of features, from which we can build a matrix

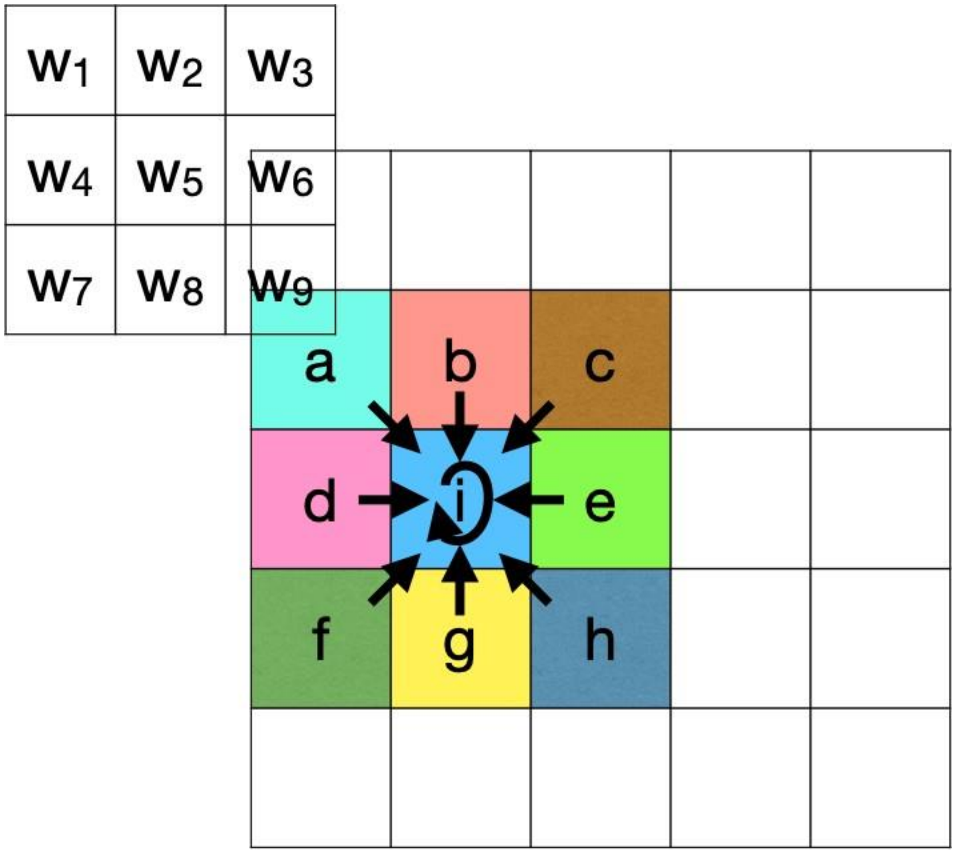
Extending Convolutions to Graphs

Recap: MLP

- $\mathbf{x} = \{1, x_1, x_2, \cdots, \}^T$
- $\mathbf{w} = \{w_0, w_1, w_2, \cdots, \}^T$
- $y_{h1} = \mathbf{w}^T\mathbf{x} = \sum_j w_j x_j = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n$
- $h_1^l = z = \sigma(y_{h1})$
- $h_1^{l+1} = \sigma(w_0^l + w_1^l h_1^l + w_2^l h_2^l + \cdots + w_n^l h_n^l)$

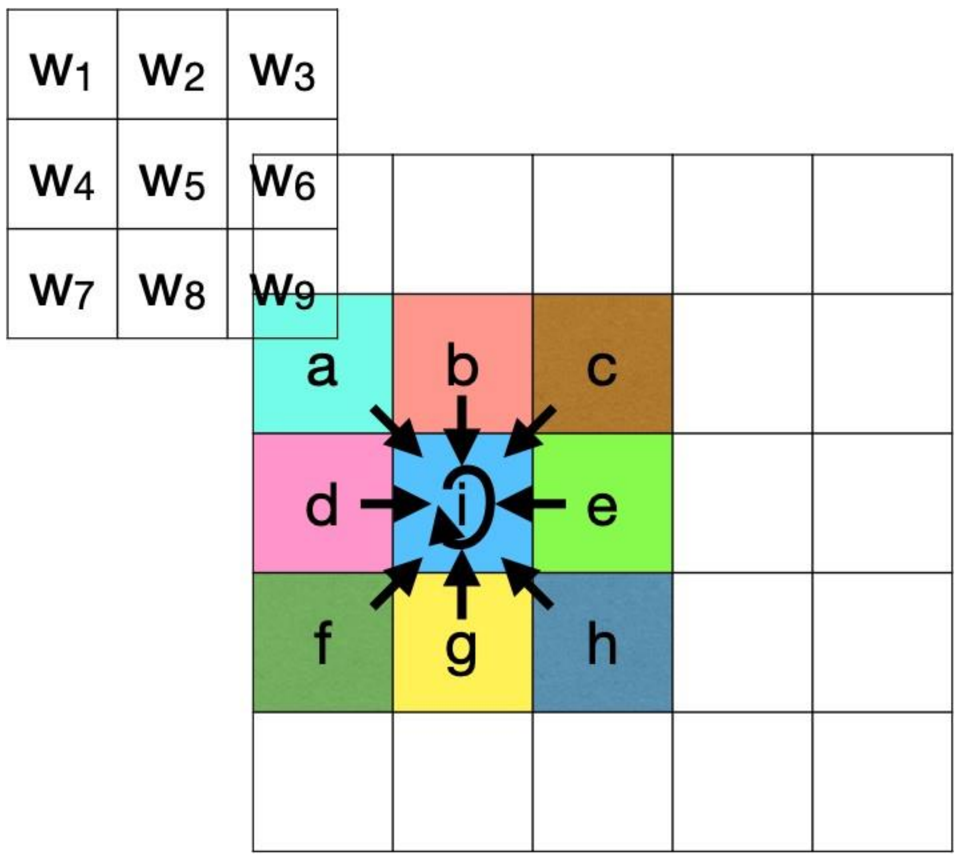


Convolution as Message Passing



Convolution as Message Passing

$$\mathbf{h}_i^{l+1} = w_1^l \mathbf{h}_a^l + w_2^l \mathbf{h}_b^l + \cdots + w_5^l \mathbf{h}_i^l + \cdots + w_9^l \mathbf{h}_h^l$$



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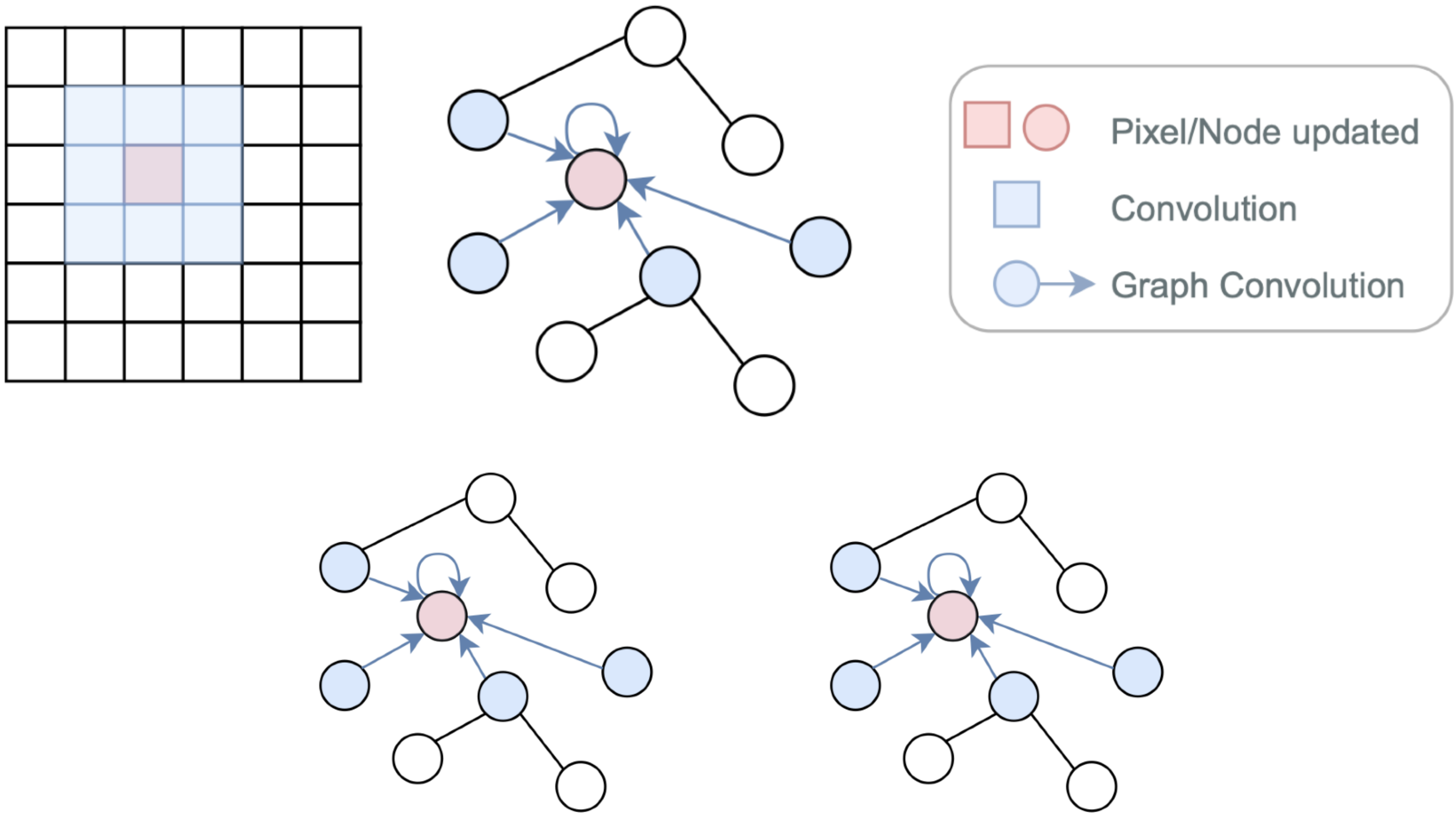

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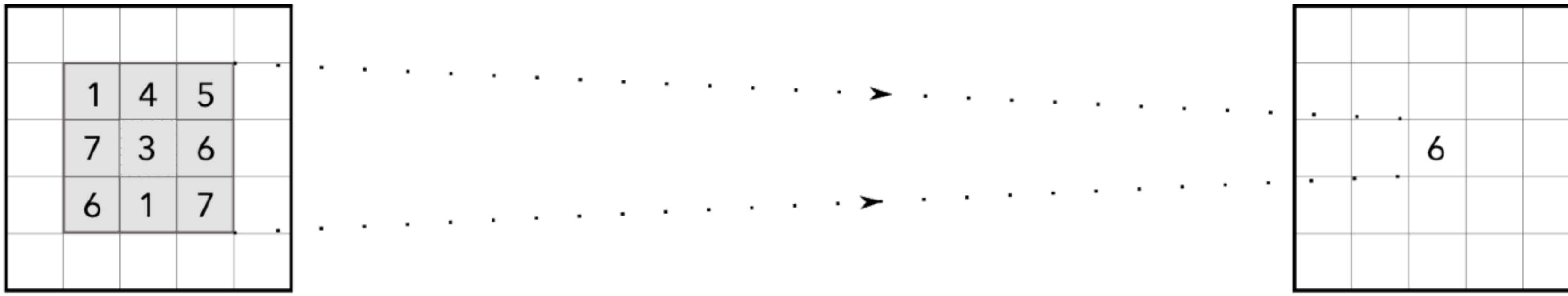
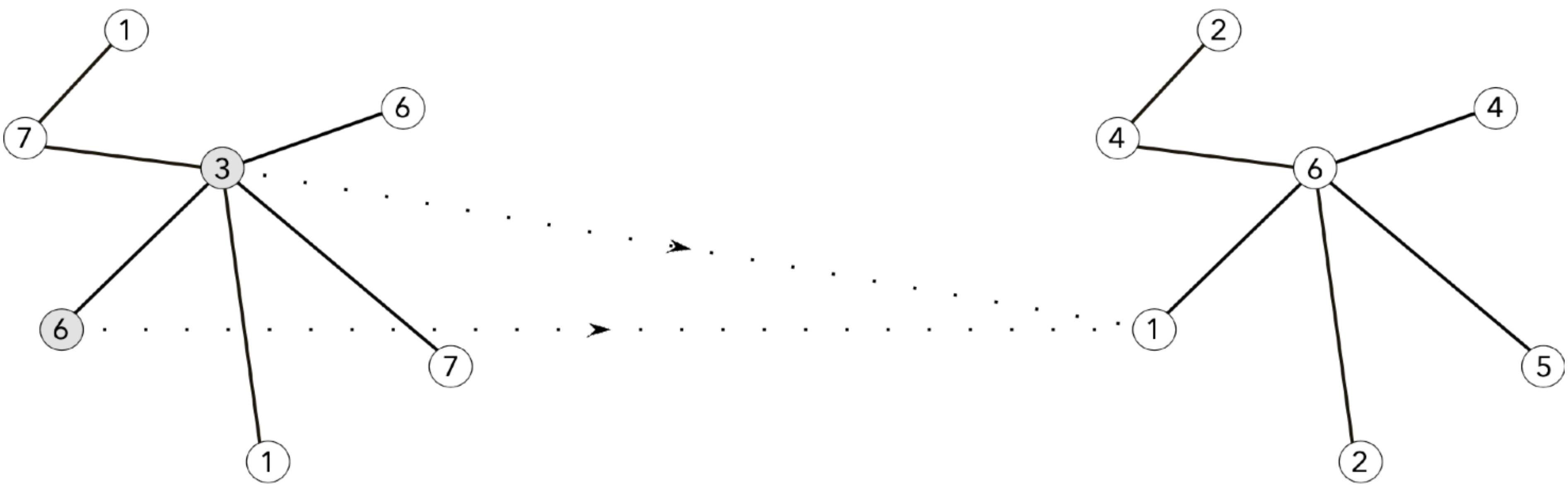
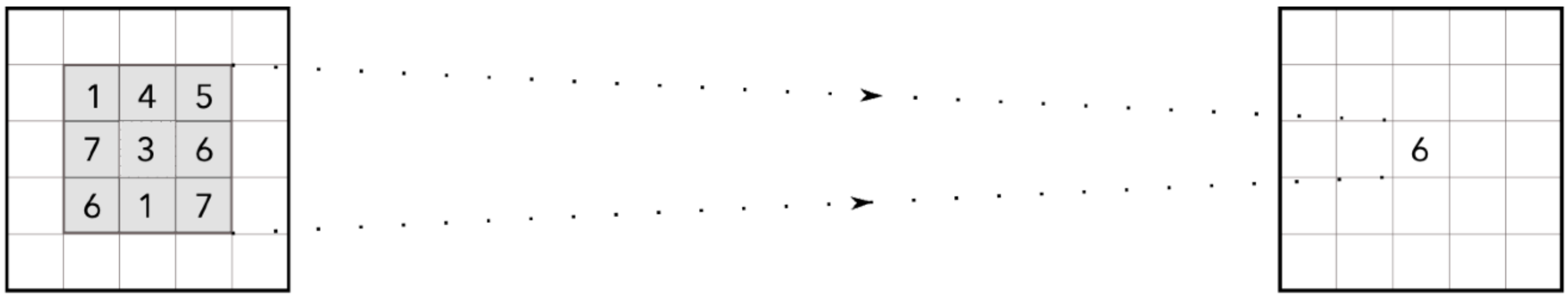


Convolution in CNNs



Localized Convolution in GNNs

Extending Convolutions to Graphs



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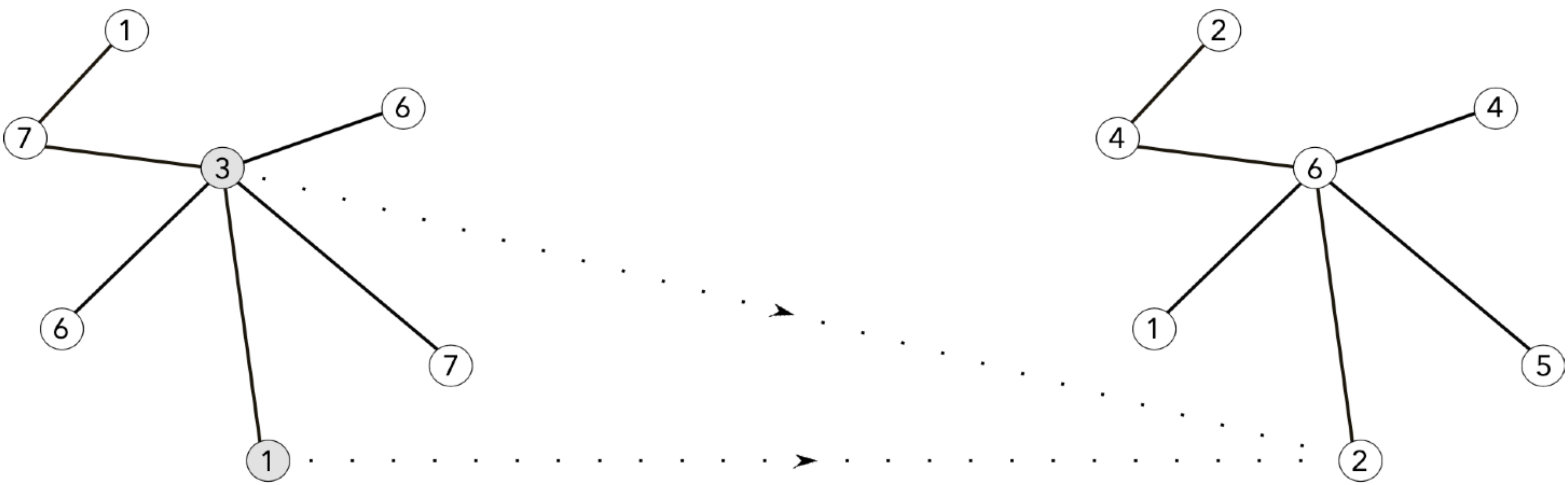
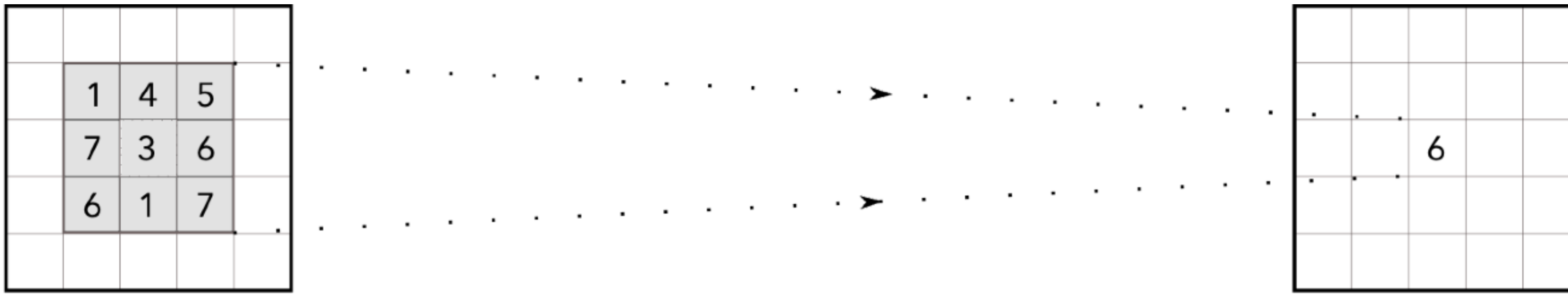


Localized Convolution in GNNs

Extending Convolutions to Graphs



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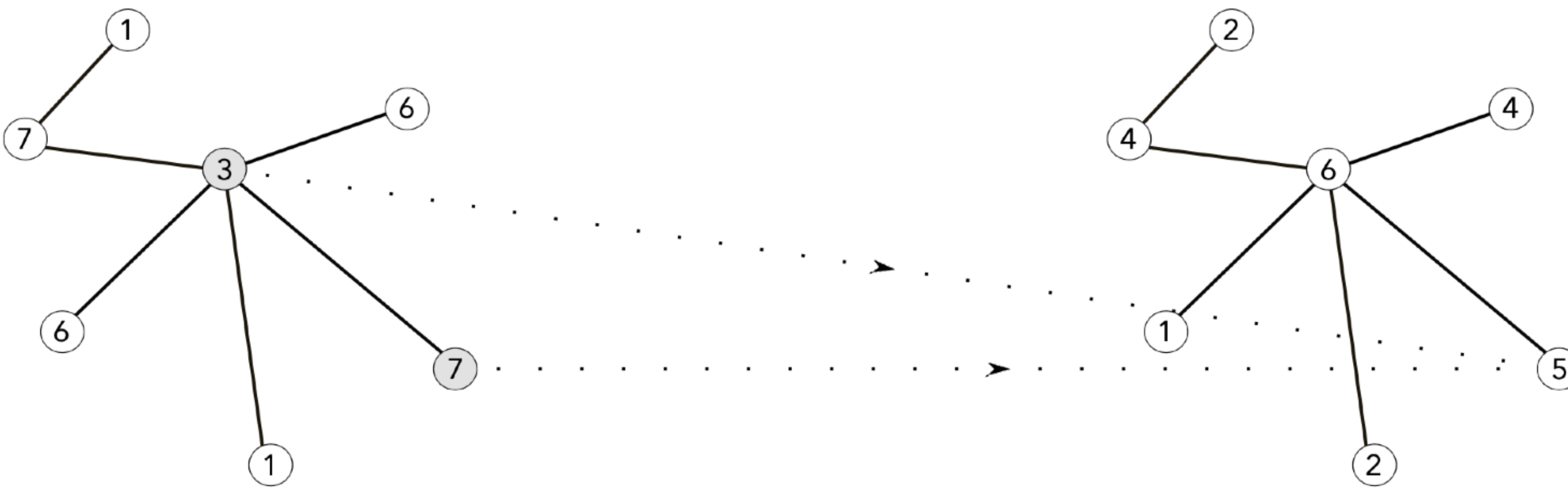

Localized Convolution in GNNs

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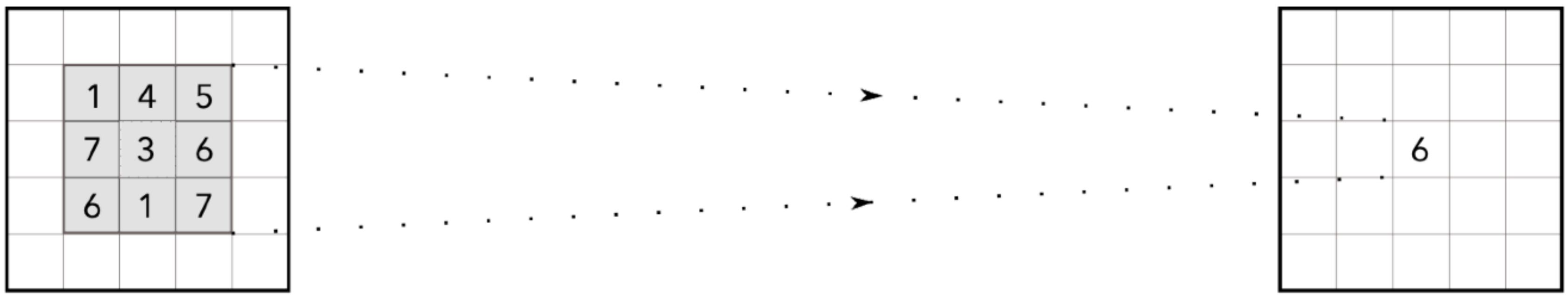

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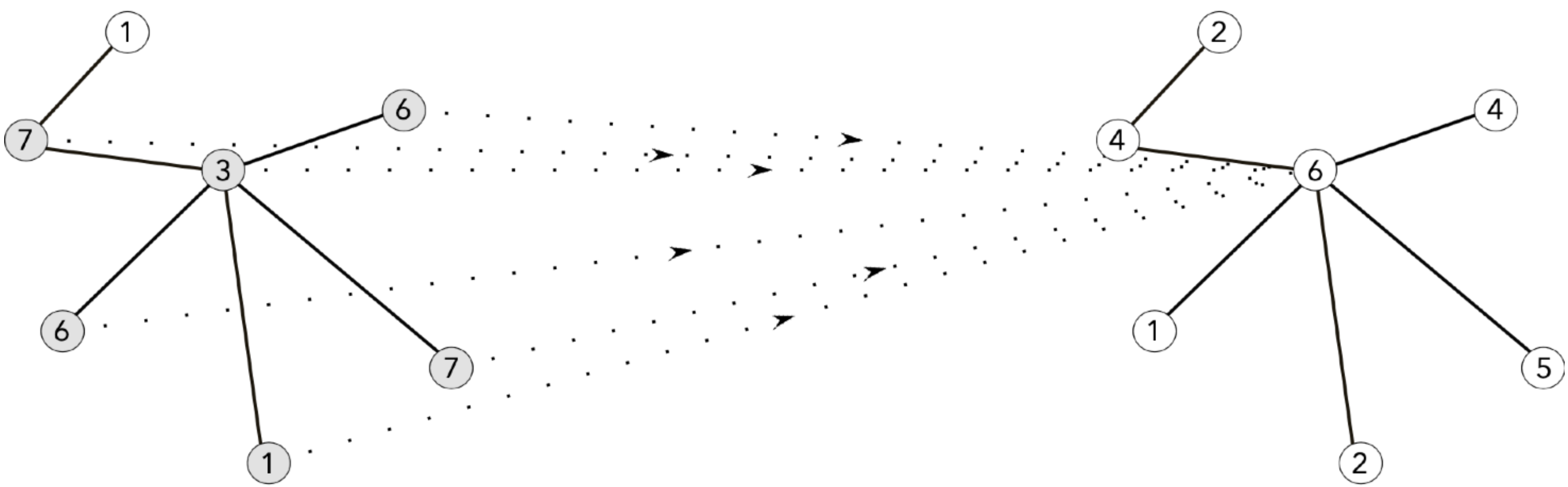
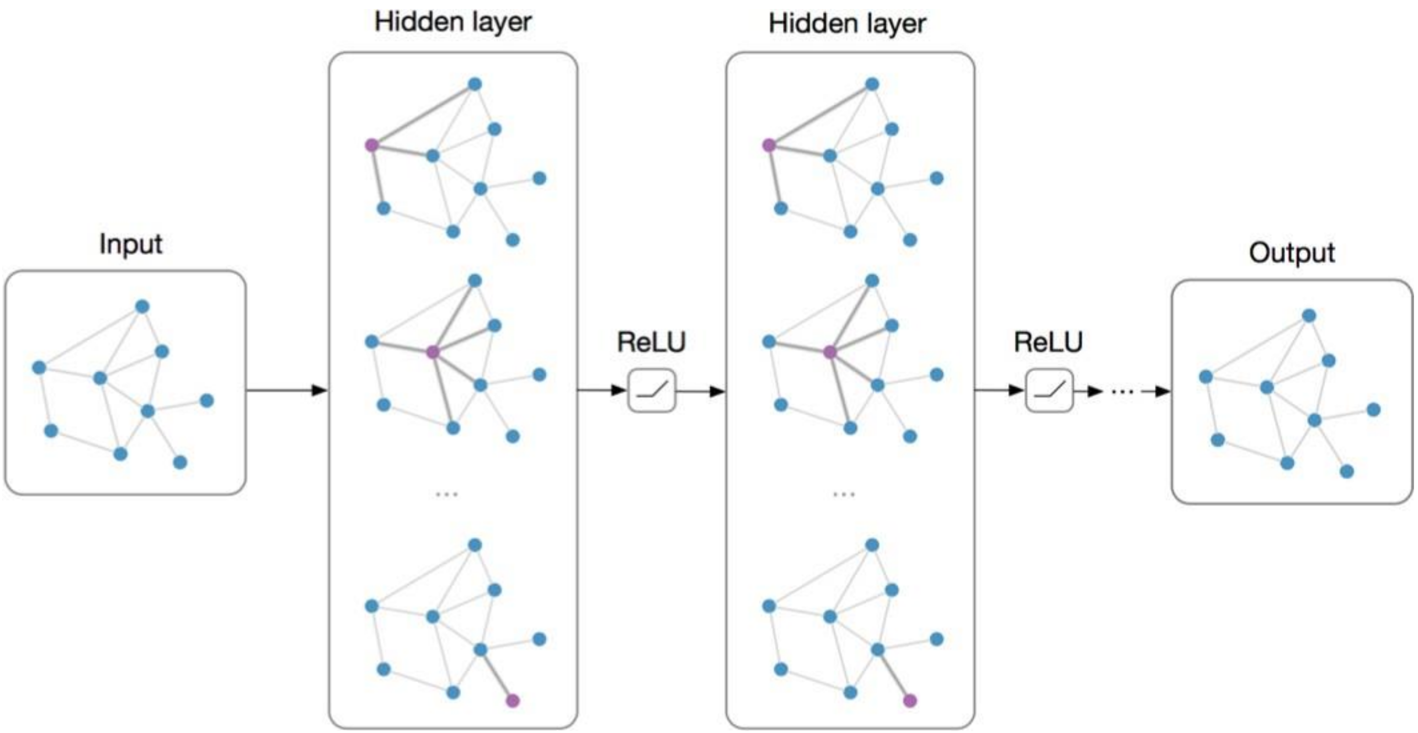
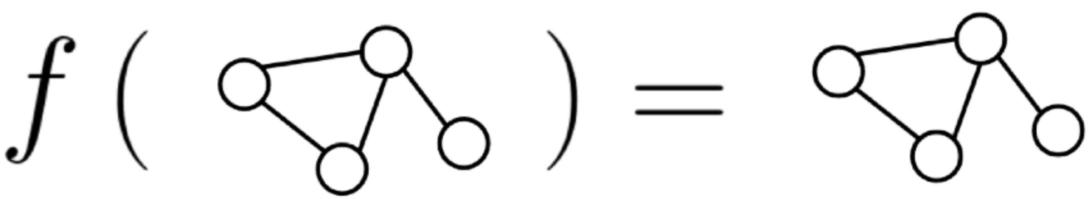


Localized Convolution in GNNs

Graph Neural Network

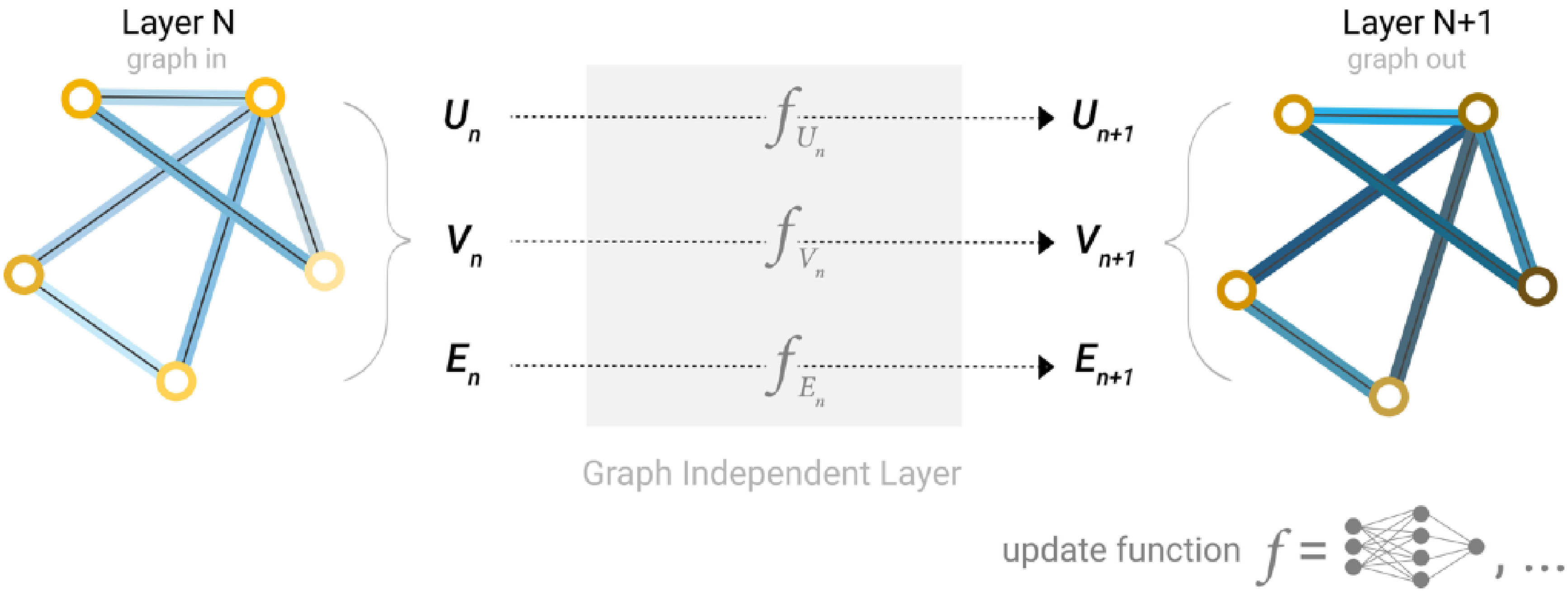
Graph Neural Network





* slide from Thomas Kipf, **University of Amsterdam**

Graph Neural Network



- GNN **does not update the connectivity** of the input graph
- Output graph of a GNN has the **same adjacency** and the **same number of feature** vectors as the input graph.
- But, the output graph has **updated embeddings**, since the GNN has updated each of the node, edge and global-context representations.

Graph Convolutional Neural Network

- Kipf and Welling (2017)

Attempt #1: $$\mathbf{h}_i^{l+1} = \sigma\left(\sum_{j \in \mathcal{N}(i)} W^l \mathbf{h}_j^l\right)$$

Graph Convolutional Neural Network

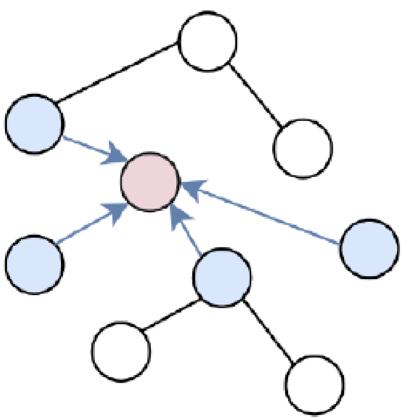
- Kipf and Welling (2017)

Attempt #1: $\mathbf{h}_i^{l+1} = \sigma\left(\sum_{j \in \mathcal{N}(i)} W^l \mathbf{h}_j^l\right)$

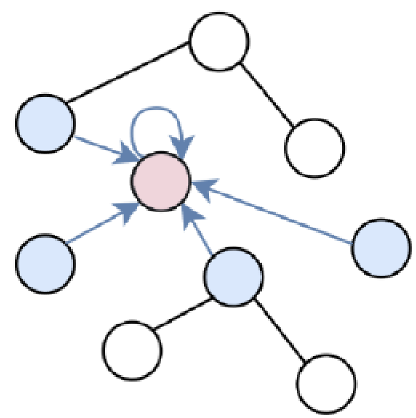
Attempt #2: $\mathbf{h}_i^{l+1} = \sigma\left(\sum_{j \in \mathcal{N}(i) \cup \{i\}} W^l \mathbf{h}_j^l\right)$

Normalised propagation matrices

- The GC layer remains valid if we replace the adjacency matrix with another matrix having the same sparsity pattern (i.e., 0 for pairs of nodes not connected).
  - Adjacency matrix with self-loops: $\hat{A} = A + I$ and $[\hat{D}]_{i,i} = \sum_j \hat{A}_{ij}$.
  - Normalised adjacency matrix (with or without self-loops): $L = D - A$ or $L = \hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}$



Without self-loop



With self-loop

  - Some of these matrices can have better properties when training.

Graph Convolutional Neural Network

- Kipf and Welling (2017)

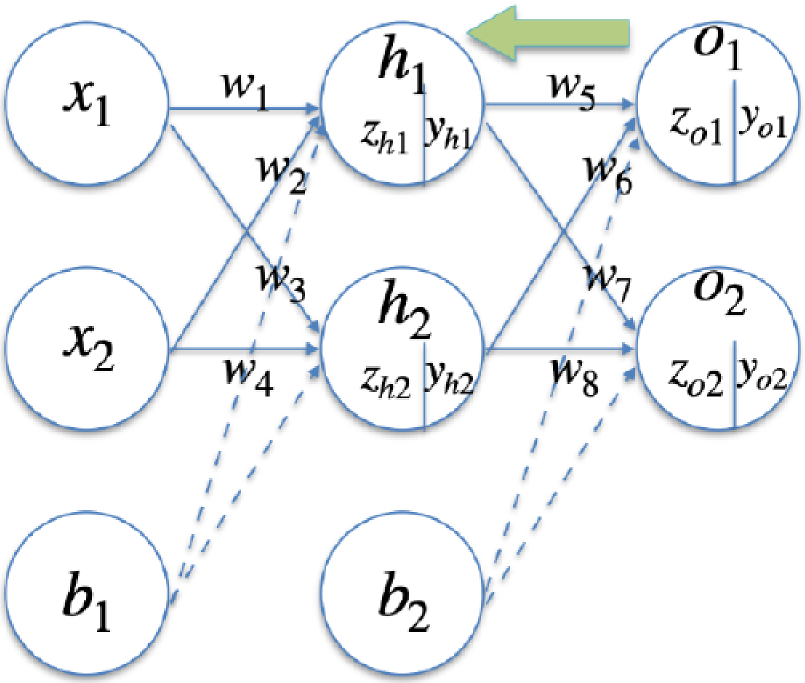
Attempt #1: $\mathbf{h}_i^{l+1} = \sigma\left(\sum_{j \in \mathcal{N}(i)} W^l \mathbf{h}_j^l\right)$

Attempt #2: $\mathbf{h}_i^{l+1} = \sigma\left(\sum_{j \in \mathcal{N}(i) \cup \{i\}} W^l \mathbf{h}_j^l\right)$

Attempt #3: $\mathbf{h}_i^{l+1} = \sigma\left(\sum_{j \in \mathcal{N}(i) \cup \{i\}} \frac{1}{\sqrt{|\mathcal{N}(i)| + 1}\sqrt{|\mathcal{N}(j)| + 1}} W^l \mathbf{h}_j^l\right)$

Recap: MLP

- $\mathbf{x} = \{1, x_1, x_2, \cdots, \}^T$
- $\mathbf{w} = \{w_0, w_1, w_2, \cdots, \}^T$
- $z = \sigma(\mathbf{w}^T \mathbf{x})$
- $H^1 = f(X, W)$
- $H^{l+1} = f(H^l, W)$



Graph Layer

- We consider graph layers of the form

$$f(X, A, W) = (H, A)$$

- acting on the node features, but keeping the connectivity the same. For simplicity, we can omit the second output and write

$$H = f(X, A, W)$$

A convolution-like operation for graphs

- A graph convolutional (GC) layer is defined as:

$$[H]_i = \phi\Big(\sum_{i \in \mathcal{N}_i} A_{ij} W^T \mathbf{x}_j \Big),$$

- which can be written compactly as:

$$H = \phi(AXW)$$

- The GC layer is easily composable into a multi-layered architecture, e.g., with two layers:

$$f(X, A) = \phi(A\phi(AXW)Z)$$
$$H^{l+1} = \phi(AH^l W^l)$$

https://www.sscardapane.it/assets/files/nnds2021/Lecture_6_graphs.pdf

A convolution-like operation for graphs

- The GC layer can be understood as a sequence of three operations:
  - 1. A local **node-wise** operation $\hat{\mathbf{x}}_i = W^T \mathbf{x}_i$.
  - 2. An aggregation with respect to the neighbourhood. This is called the **message-passing** phase.
  - 3. A standard non-linearity.

- In an image convolution, points (1)-(2) are combined in the filtering operation, because each pixel has a fixed neighbourhood. Here, this is not possible because we cannot easily initialise trainable parameters to weight the neighbourhood.

Summary / Recap

Graph

- A graph is a pair $G = (V, E)$, where $V = \{1, \cdots, n\}$ is a set of n vertices (nodes), and $E = \{(i, j) \mid i, j \in N\}$ is a set of edges between them.
- Adjacency matrix A where: $A_{ij} = \begin{cases} 1 & \text{if } (i, j) \in E \\ 0 & \text{otherwise} \end{cases}$
- If $A^T = A$, we say the graph is undirected.
- Neighbourhood $\mathcal{N}_i = \{j \mid A_{ij} = 1\}$
- Degree $[D]_{i,i} = \sum_j A_{ij}$
- Adjacency matrix with self-loops: $\hat{A} = A + I$ and $[\hat{D}]_{i,i} = \sum_j \hat{A}_{ij}$.
- Normalised adjacency matrix / Laplacian: $L = D - A$ or $L = \hat{D}^{-1/2} \hat{A} \hat{D}^{-1/2}$

A convolution-like operation for graphs

- A graph convolutional (GC) layer is defined as:

$$[H]_i = \phi\Big(\sum_{i \in \mathcal{N}_i} A_{ij} W^T \mathbf{x}_j\Big),$$

- which can be written compactly as:

$$H = \phi(AXW)$$

- The GC layer is easily composable into a multi-layered architecture, e.g., with two layers:

$$f(X, A) = \phi(A\phi(AXW)Z)$$
$$H^{l+1} = \phi(AH^l W^l)$$

How do we use GNN / GCN for real problems?

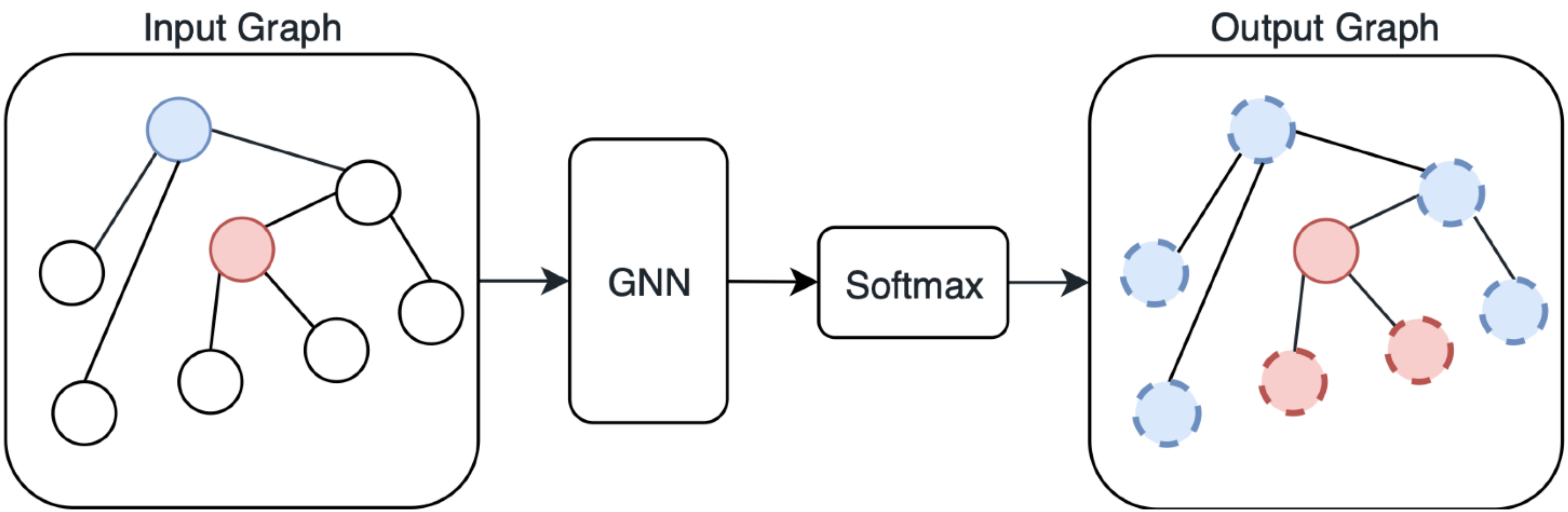
GNN Tasks

- **Node Classification**: label data samples by taking into account their neighbours.

- **Link Prediction**: predict most likely links in the graph.

Task #1: Node classification

- For the node classification, we can stack two graph convolutional layer to form a Graph Neural Network. A softmax() applied on each node embedding of the last layer will provide the prediction y.



Kipf, T.N. and Welling, M., 2016. Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907

Task #1: Node classification

- Suppose a subset $\mathcal{T} \subset \mathcal{N}$ of nodes has a known class y (e.g., fake or certified users in a social network). We can use a GCN to classify all the nodes of the graph simultaneously:

$$\hat{Y} = \text{softmax}(A\varphi(AXW)Z)$$

- We optimise the weights of the network with gradient descent:

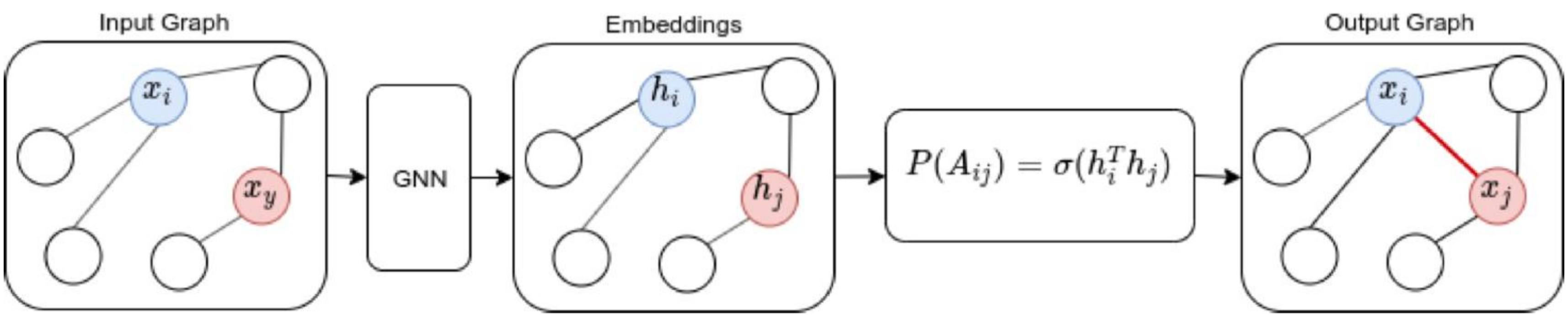
$$W^*, Z^* = \arg\min \frac{1}{|\mathcal{T}|} \sum_{i \in \mathcal{T}} \text{cross-entropy}(y_i, \hat{y}_i) \, .$$

Kipf, T.N. and Welling, M., 2016. Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907

Task #2: Link Prediction

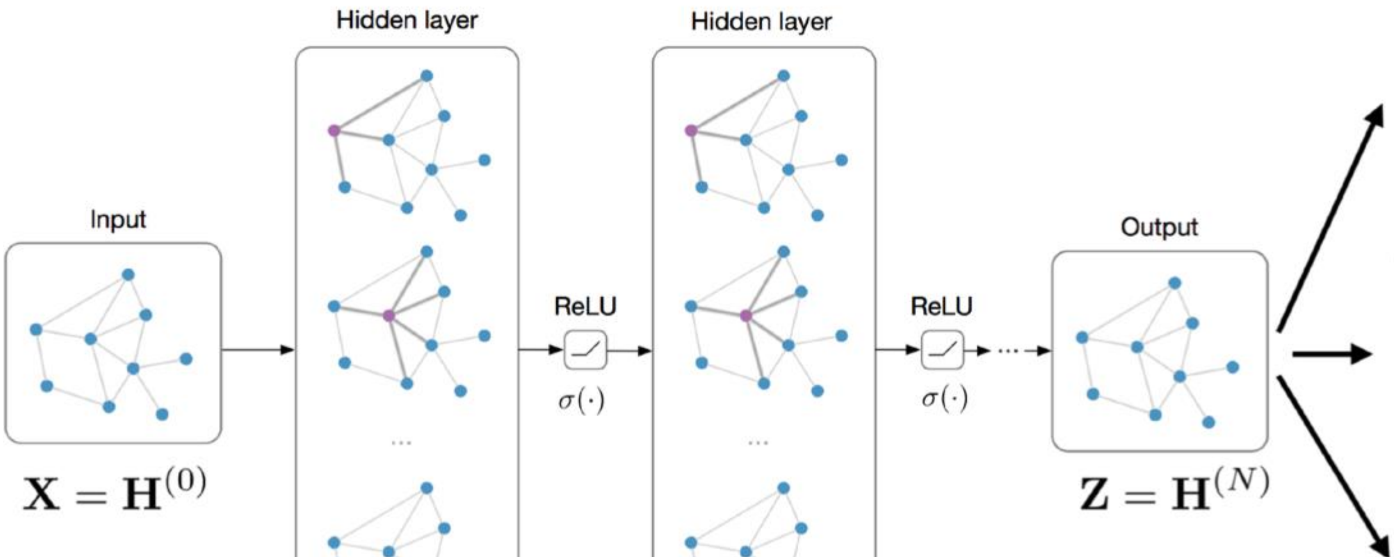
- In link prediction, the objective is to predict whether two nodes in a network are likely to have a link.

- We can get the probability for each edge by taking the inner product of the embedding produced by a GNN.



- Also, in this case the model is optimised by minimising the **cross-entropy loss** function.

Node classification, Graph Classification, Link Prediction



$$\mathbf{H}^{(l+1)} = \sigma\left(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}^{(l)}\right)$$

Node classification:

$$\mathrm{softmax}(\mathbf{z_n})$$

e.g. Kipf & Welling (ICLR 2017)

Graph classification:

$$\mathrm{softmax}(\textstyle\sum_n \mathbf{z_n})$$

e.g. Duvenaud et al. (NIPS 2015)

Link prediction:

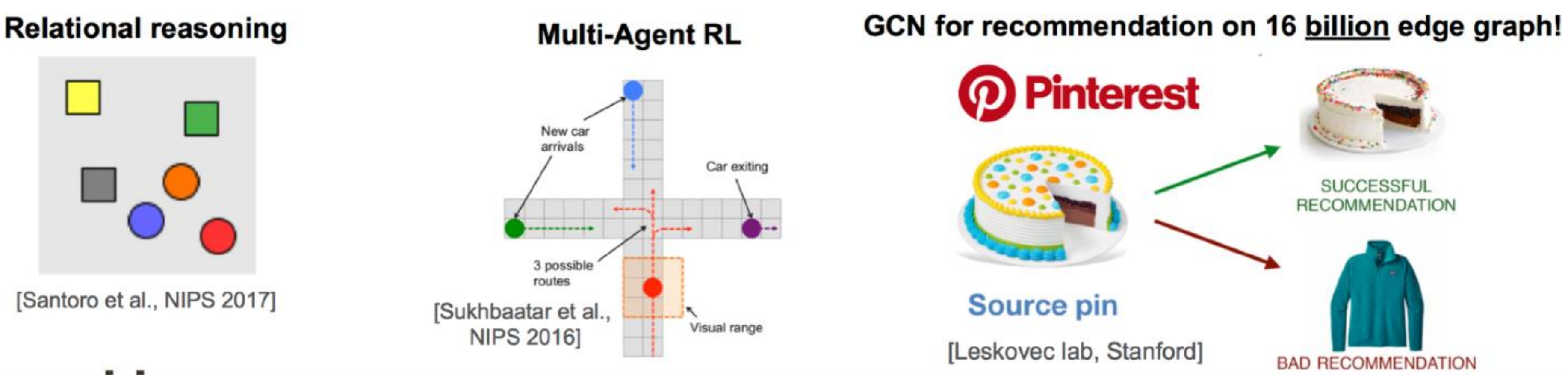
$$p(A_{ij}) = \sigma(\mathbf{z_i^T z_j})$$

Kipf & Welling (NIPS BDL 2016)
"Graph Auto-Encoders"

https://www.cs.ubc.ca/~lsigal/532S_2018W2/Lecture18a.pdf

Conclusions

- Deep learning on graphs works and is very effective!
- Exciting area: lots of new applications and extensions (hard to keep up)



Conclusions

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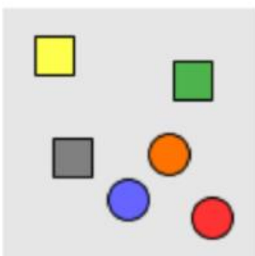
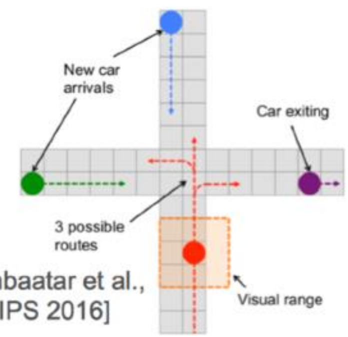
- Exciting area: lots of new applications and extensions (hard to keep up)

Relational reasoning



[Santoro et al., NIPS 2017]

Multi-Agent RL



[Sukhbaatar et al., NIPS 2016]

GCN for recommendation on 16 billion edge graph!

[Leskovec lab, Stanford]

- Open problems:
  - Theory
  - Scalable, stable generative models
  - Learning on large, evolving data
  - Multi-modal and cross-model learning (e.g., sequence2graph)

Software Libraries

- Multiple libraries build on standard deep learning frameworks to provide GNN functionalities:
  - Deep Graph Library (framework agnostic, very scalable):
  - https://www.dgl.ai/

  - PyTorch Geometric (great for reproducing results):
  - https://github.com/pyg-team/pytorch_geometric

  - Spektral (TensorFlow, smaller than the other two):
  - https://graphneural.network/