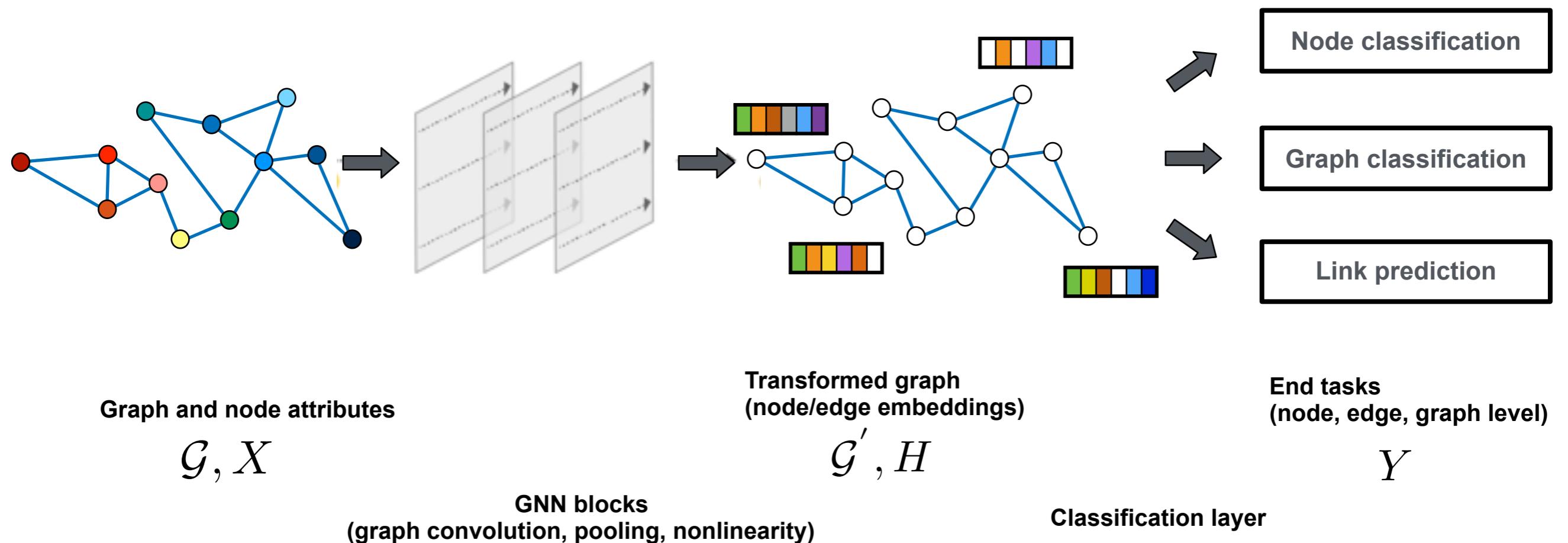


Graph neural networks: State-of-the-art architectures

Dr Dorina Thanou
April 8, 2025

Recap: Graph neural networks (GNNs)

- A different way of obtaining ‘deeper’ embeddings inspired by deep learning
- They generalize to graphs with node attributes



Recap of previous lecture

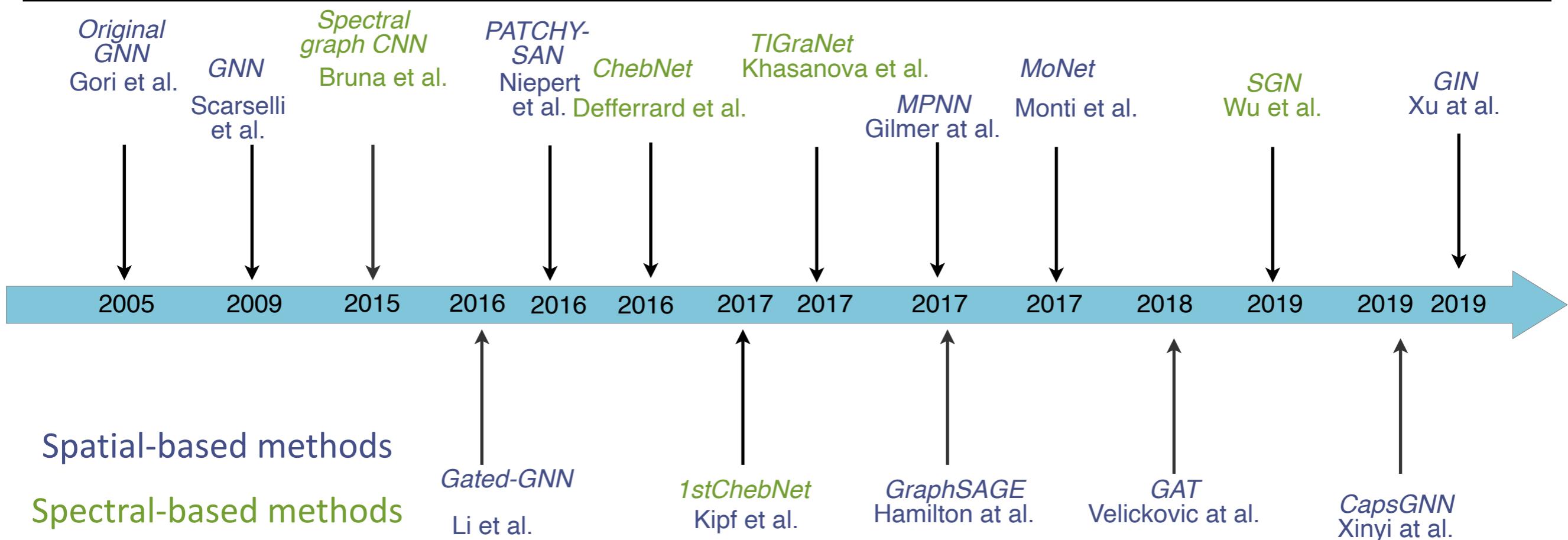
- Graph neural networks are designed based on a generalization of deep learning techniques on graphs
- Their key ingredients are:
 - Parameter sharing across nodes
 - Local exchange of information and neighbourhood aggregation on the graph (e.g., graph convolution)
 - Graph subsampling/pooling (mainly used for graph level tasks)
- Two different ways of defining graph convolution:
 - A spectral viewpoint
 - A spatial viewpoint

Outline

- State-of-the-art GNN architectures

- Spectral approaches
- Spatial approaches

First GNN architectures



- Recent trends
 - Spectrally-inspired architectures: GraphHeat (Xu'19), GWNN (Xu'19), SIGN (Frasca'20), DGN (Beaini'20), Framelets (Zheng'21), FAGCN (Bo'21)
 - More expressive GNNs: higher order WL test (Maron'19, Morris'20), physics-inspired GNNs (Chamberlain'21), and many more!

Outline

- State-of-the-art GNN architectures

- **Spectral approaches**
- Spatial approaches

Spectral approaches in one slide

- Convolution is defined in the graph Fourier domain (see previous lecture)

$$x *_{\theta} g = \chi \hat{g}(\theta) \chi^T x$$

- Spectral GCNN:**

$$\hat{g}(\lambda) = \theta \quad \longrightarrow \quad x * g = \chi \theta \chi^T x$$

- ChebNet:**

$$\hat{g}(\lambda) = \sum_{k=0}^K \theta_i T_i(\lambda) \quad \longrightarrow \quad x * g = \sum_{k=0}^K \theta_i T_i(L) x$$

- GCN:**

$$K = 1 \quad \longrightarrow \quad x * g = (\theta_0 - \theta_1 D^{-1/2} W D^{-1/2}) x$$

- Parameters θ are learned through the network

Spectral GCNN

- **Main intuition:** Define graph convolutional filters in the spectral domain

$$x * g = \chi \hat{g}(\Lambda) \chi^T x = \hat{g}(L)x$$

- A GCNN is defined as a series of spectral convolutional layers:

$$h^{l+1} = \sigma(\chi \theta^{l+1} \chi^T h^l)$$

Non-linearity

- $\theta^{l+1} = \text{diag}(\theta_{\lambda_1}, \theta_{\lambda_2}, \dots, \theta_{\lambda_N})$ are **learnable spectral coefficients** in each layer
- First spectral graph CNN architecture
- $O(N)$ parameters per layer
- $O(N^2)$ for the computation of the GFT, IGFT
- Filters are eigenbasis dependent: they do not generalize across graphs

[Bruna et al., Spectral Networks and Deep Locally Connected Networks on Graphs, ICLR 2014]

Parametrized spectral graph filters

- **Main intuition:** Represent **spectral filters with polynomials** of the Laplacian

$$\widehat{g^{l+1}}(\lambda) = \sum_{k=0}^K \theta_k^{l+1} \lambda^k$$

- Monomials:

$$h^{l+1} = \sigma(\widehat{g^{l+1}}(L)h^l) = \sigma\left(\sum_{k=0}^K \theta_k^{l+1} L^k h^l\right) = \sigma\left(\sum_{k=0}^K \theta_k^{l+1} z_k\right)$$

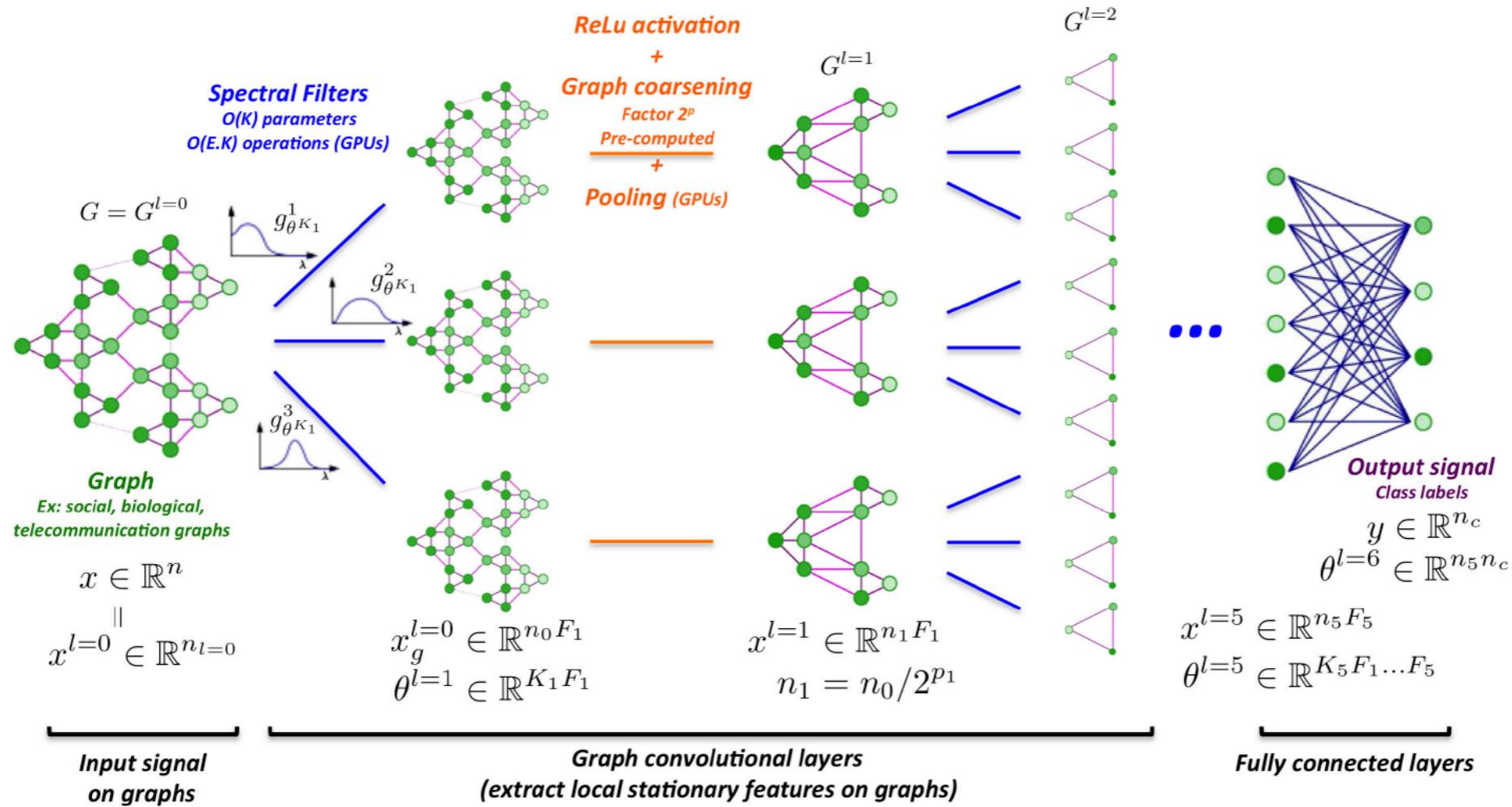
- with $z_0 = 1, z_1 = Lh^l, \dots, z_{k+1} = Lz_k$

- Chebyshev polynomials:

$$h^{l+1} = \sigma(\widehat{g^{l+1}}(L)h^l) = \sigma\left(\sum_{k=0}^K \theta_k^{l+1} T_k(L)h^l\right) = \sigma\left(\sum_{k=0}^K \theta_k^{l+1} z_k\right)$$

- with $z_0 = 1, z_1 = Lh^l, \dots, z_{k+1} = 2Lz_k - z_{k-1}$

ChebNet



- Coefficients of polynomials are learnable; $O(1)$ parameters per layer
- Filters have K-hops support
- No explicit computation of the eigenvectors of the Laplacian

[Defferrard et al., Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering, NeurIPS 2016]

Graph Convolutional Networks (GCN)

- **Main intuition:** Design a scalable architecture with **first-order approximation** of spectral graph convolution

$$\begin{aligned} g * x &\approx \theta_0 x + \theta_1 (L - I_N) x = \theta_0 x - \theta_1 D^{-1/2} \boxed{W D^{-1/2}} x \\ &\quad \downarrow \quad \theta = \theta_0 = -\theta_1 \\ g * x &\approx \theta(I + D^{-1/2} W D^{-1/2}) x \\ &\quad \downarrow \quad \tilde{W} = W + I_N \\ g * x &\approx \theta \tilde{D}^{-1/2} \tilde{W} \tilde{D}^{-1/2} x \end{aligned}$$

Adjacency/Weight matrix
Degree matrix

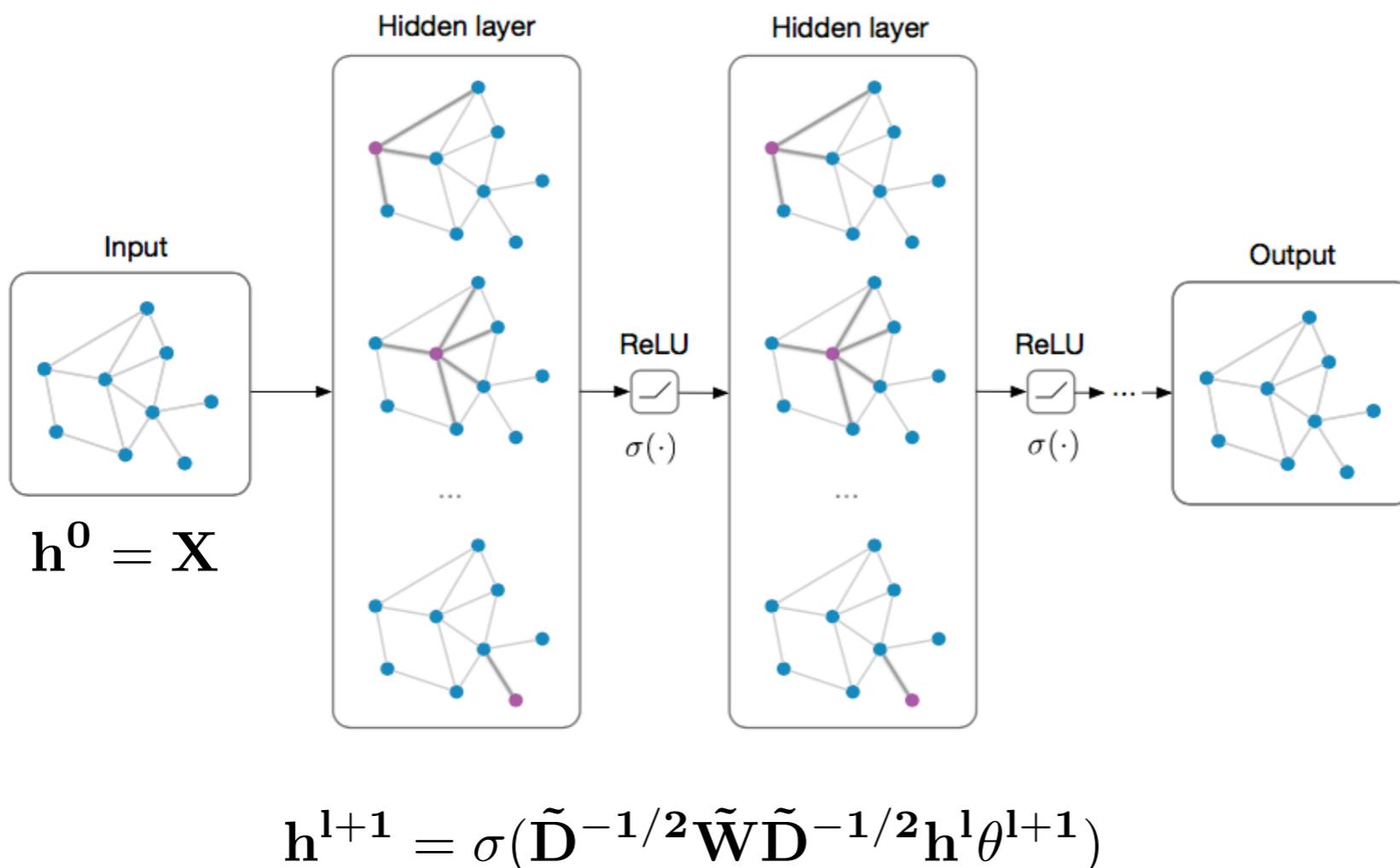
- A convolutional layer is defined as:

$$h^{l+1} = \sigma(\tilde{D}^{-1/2} \tilde{W} \tilde{D}^{-1/2} h^l \boxed{\theta^{l+1}})$$

Learned parameters

GCN architecture

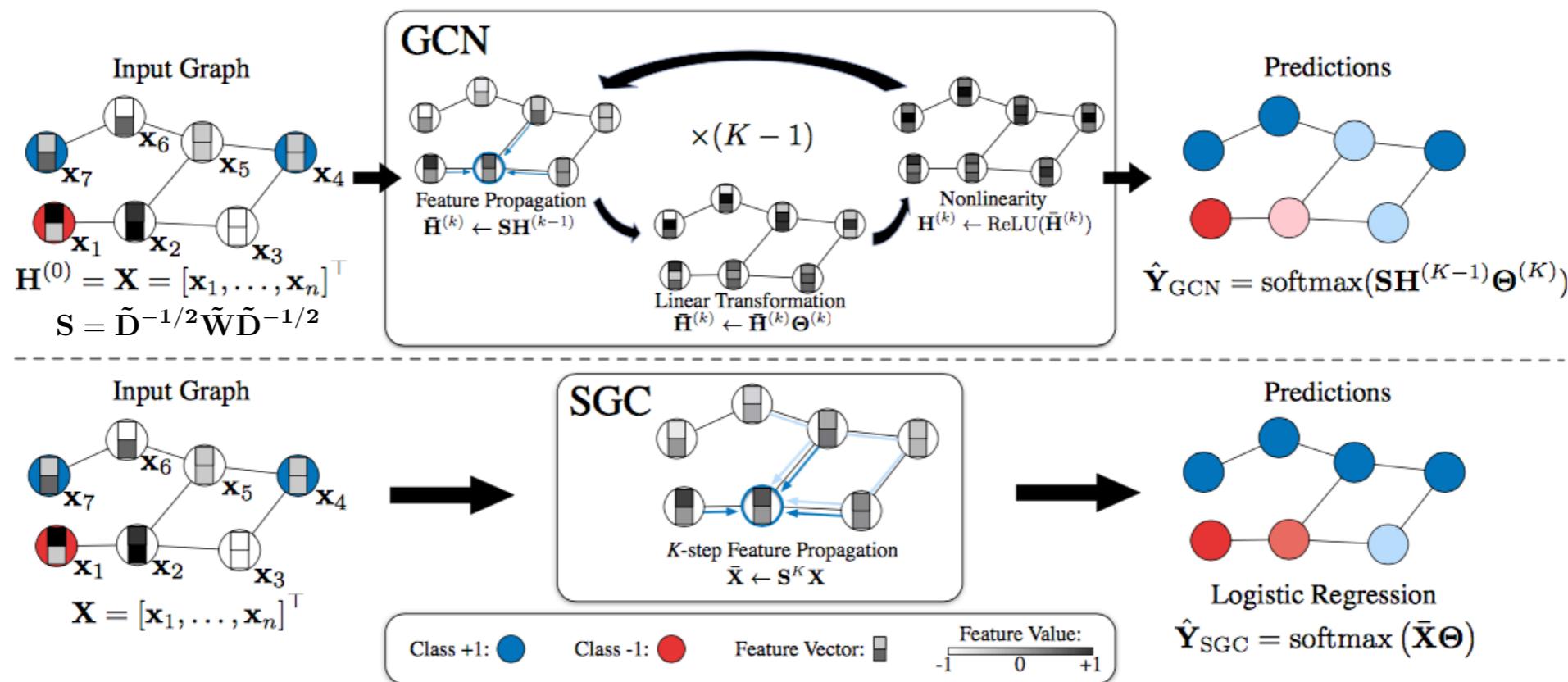
- Very often, it consists of two GCN layers



[Kipf et al., Semi-Supervised Classification with Graph Convolutional Networks, ICLR, 2017]

Simple Graph Convolution (SGC)

- **Main intuition:** Reduce further the complexity of GCN by removing nonlinearities



- Reduces the procedure to a simple low pass filtering
- No significant loss in the performance

[Wu et al., Simplifying Graph Convolutional Networks, ICML 2019]

Summary of spectral methods

- **Pros:**

- Clear intuition from the spectral domain
- They take into account the global structure of the graph

- **Cons:**

- Generalization is an open research question

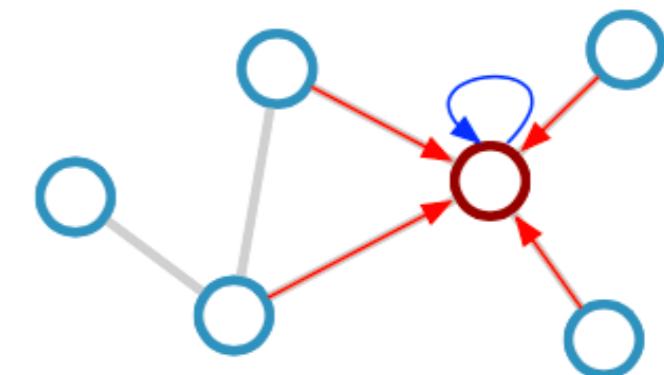
Outline

- State-of-the-art GNN architectures
 - Spectral approaches
 - **Spatial approaches**

Spatial approaches in one slide

- Generate node embeddings based on local neighborhoods
 - Nodes aggregate information from their neighbors using a permutation-invariant function
 - The feature vector of each node is updated based on its current values and the aggregated neighbourhood representation
- Feed the embeddings into a loss function (usually task specific)
- **Key difference between architectures:** How nodes aggregate information across layers

$$h_i^{l+1} = \sigma(U^l h_i^l + M^l \sum_{j \in \mathcal{N}_i} h_j^l)$$

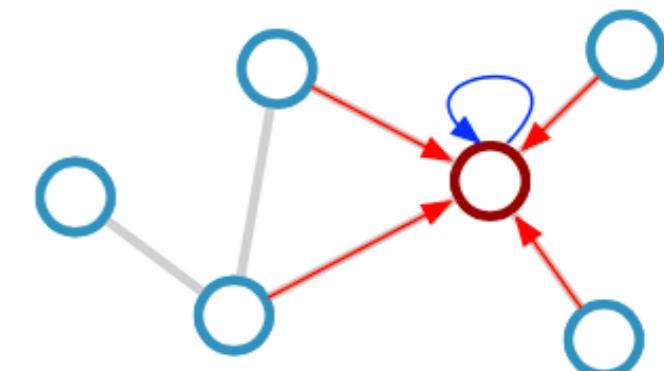


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Trainable parameters



Message Passing Neural Network (MPNN)

- **Main intuition:** Each node exchange messages with its neighbors and update its representations based on these messages
- The message passing scheme runs for T time steps and updates the representation of each vertex based on its previous representation and the representation of its neighbors

$$m_i^{l+1} = \sum_{j \in \mathcal{N}_i} M_l(h_i^l, h_j^l, e_{ij}) \quad \text{Message function}$$
$$h_i^{l+1} = U_l(h_i^l, m_i^{l+1}) \quad \text{Vertex update function}$$

Learned differentiable functions!

[Gilmer et al, Neural Message Passing for Quantum Chemistry, ICML, 2017]

MPNN - Example

- At each iteration, the embeddings are updated as follows:

$$h_1^{l+1} = \theta_0^l h_1^l + \theta_1^l h_2^l + \theta_1^l h_3^l$$

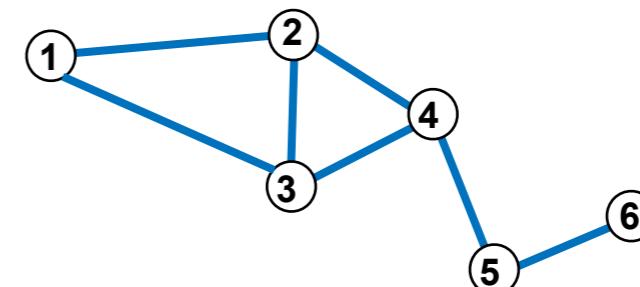
$$h_2^{l+1} = \theta_0^l h_2^l + \theta_1^l h_1^l + \theta_1^l h_3^l + \theta_1^l h_4^l$$

$$h_3^{l+1} = \theta_0^l h_3^l + \theta_1^l h_1^l + \theta_1^l h_2^l + \theta_1^l h_4^l$$

$$h_4^{l+1} = \theta_0^l h_4^l + \theta_1^l h_2^l + \theta_1^l h_3^l + \theta_1^l h_5^l$$

$$h_5^{l+1} = \theta_0^l h_5^l + \theta_1^l h_4^l + \theta_1^l h_6^l$$

$$h_6^{l+1} = \theta_0^l h_6^l + \theta_1^l h_5^l$$

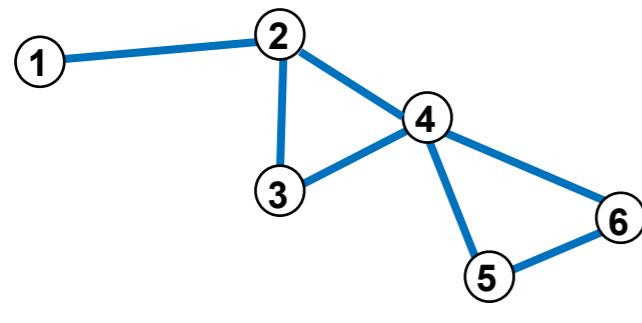


- The output of the message passing is:

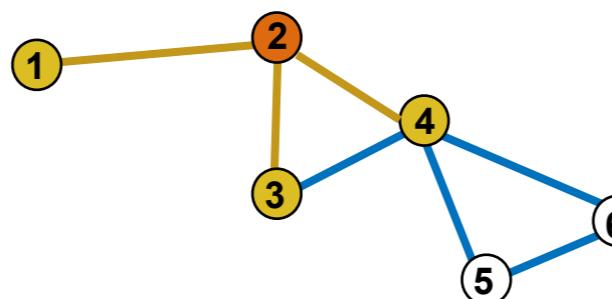
$$\{h_1^{l_{max}}, h_2^{l_{max}}, h_3^{l_{max}}, h_4^{l_{max}}, h_5^{l_{max}}, h_6^{l_{max}}\}$$

A local view of MPNNs

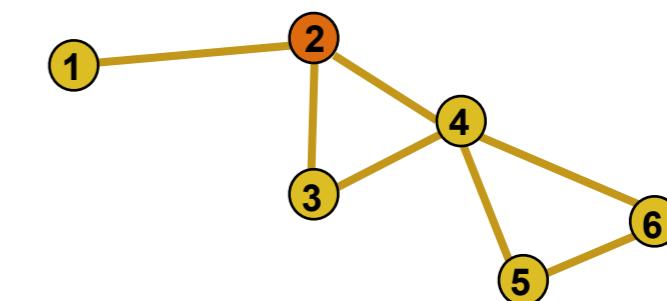
- MPNNs focus on recursive neighbourhood aggregation: they propagate messages on the edges for a fixed number of iterations layers
- After k iterations (or layers) the embedding of each node is affected by the node's k -hop neighborhood, i.e., the subgraph containing k -hops nodes



Initial graph



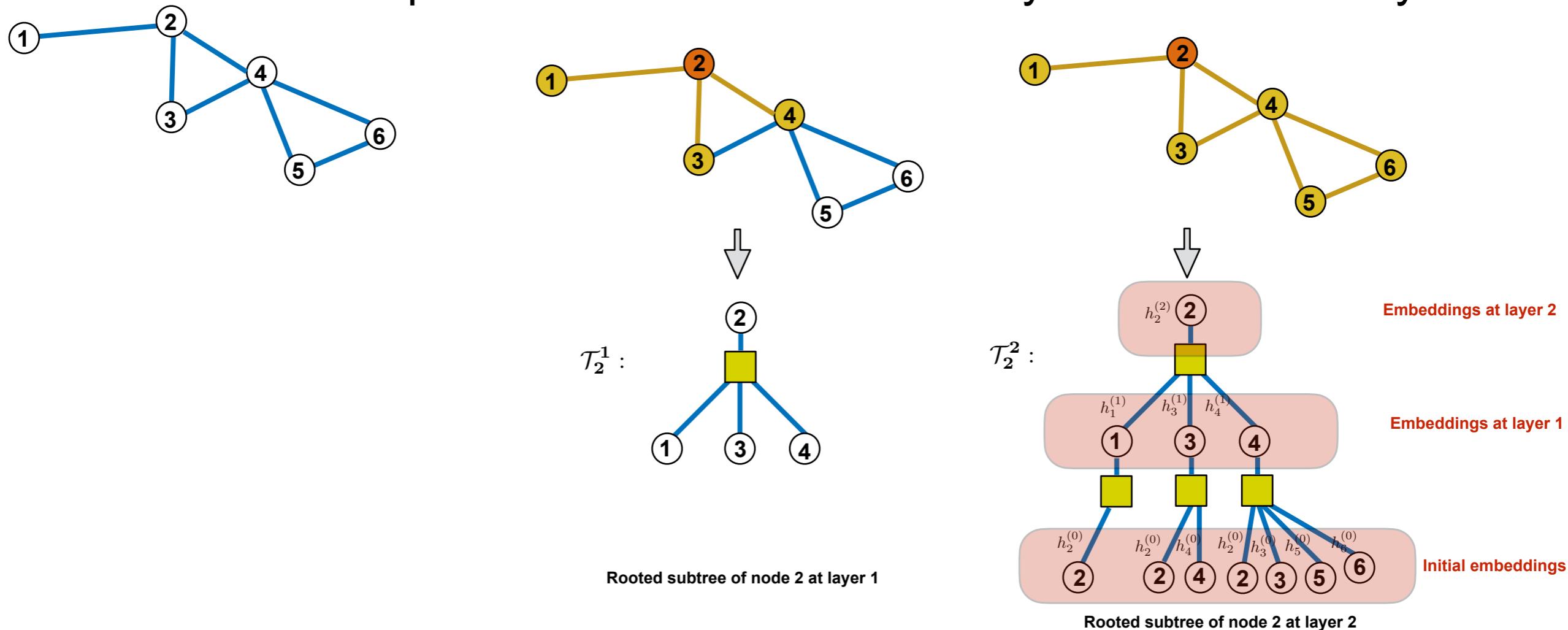
Receptive field at layer 1



Receptive field at layer 2

From graphs to rooted subtrees

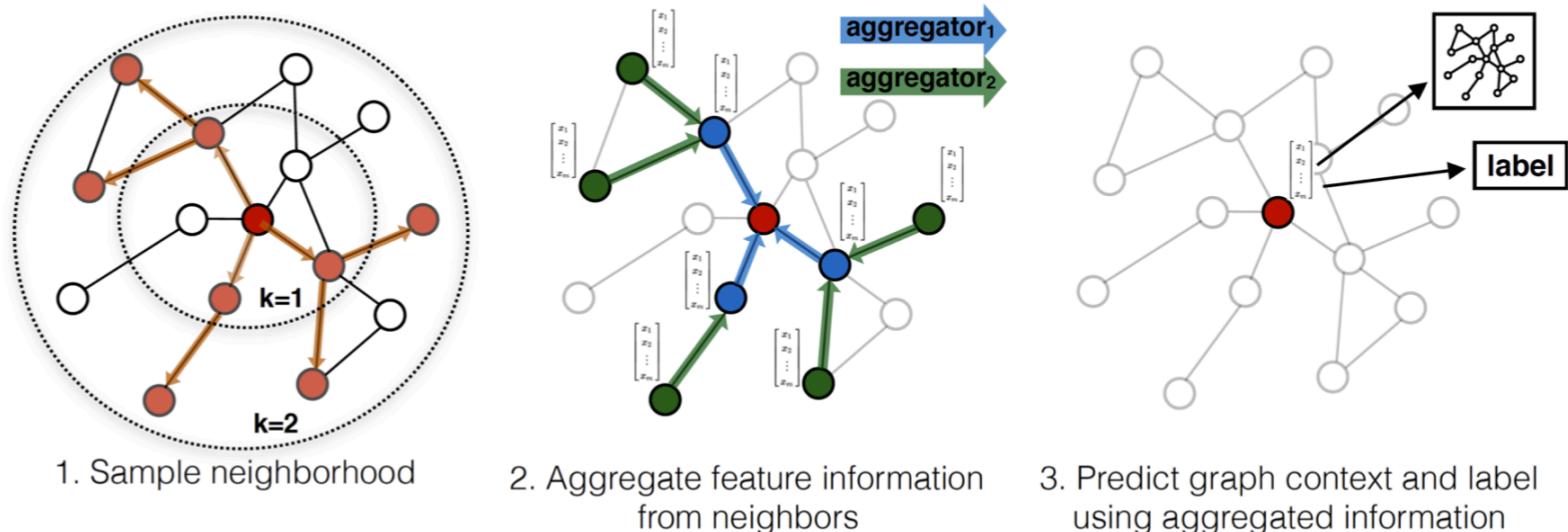
- Each subgraph can be mapped to a rooted subtree or a subtree pattern
- The maximum depth of the subtree is defined by the number of layers



Different rooted subtrees should be assigned different node embeddings!

GraphSAGE

- **Main intuition:** Subsample the neighborhood for better scalability; Node's neighborhood defines a computational graph
- Aggregate the feature information from sample neighbors
- Different loss functions: Cross entropy, Hinge,...
- Usually 2-3 layers deep

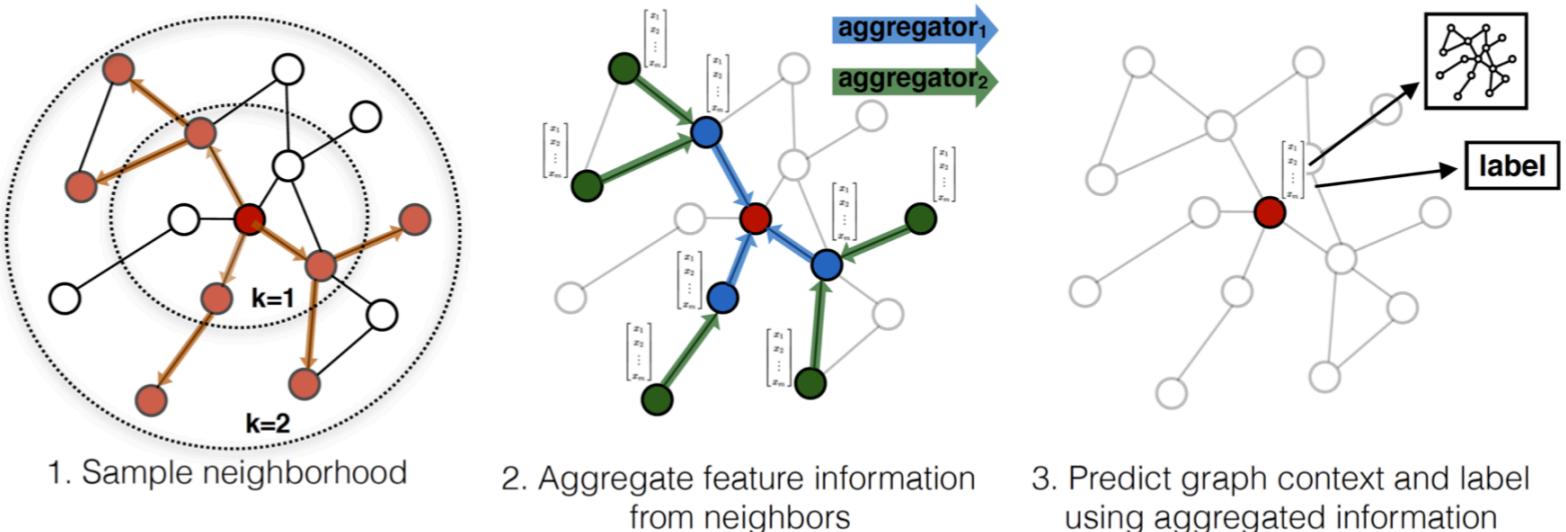


$$h_i^{l+1} = \text{ReLU}\left(\theta_0^l h_i^l, \bigoplus_{j \in \mathcal{N}_i} \text{ReLU}(\theta_1^l h_j^l)\right)$$

[Hamilton et al, Inductive Representation Learning on Large Graphs, NeurIPS, 2017]

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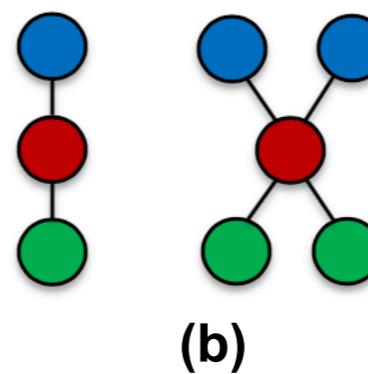
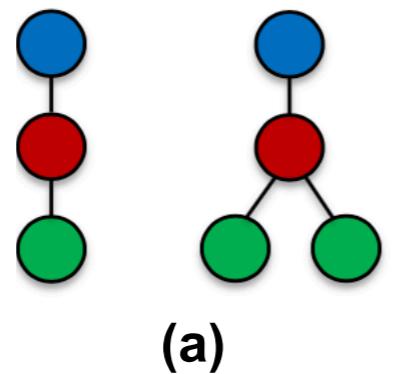
Trained aggregation function: Averaging/max pooling/LSTM

[Hamilton et al, Inductive Representation Learning on Large Graphs, NeurIPS, 2017]

Graph Isomorphism Network (GIN)

- **Main intuition:** Maximize the representation power of GNNs
 - Ensure that different rooted subtrees are mapped into different node embeddings injectively
 - Aggregation and readout functions should be injective, e.g., sum

Which aggregators can discriminate the red node?



(a) max fails; (b) max and mean fails

Sum succeeds in (a) and (b)

- GIN is a maximally-expressive GNN

- An MLP (universal approximator) can approximate an injective function

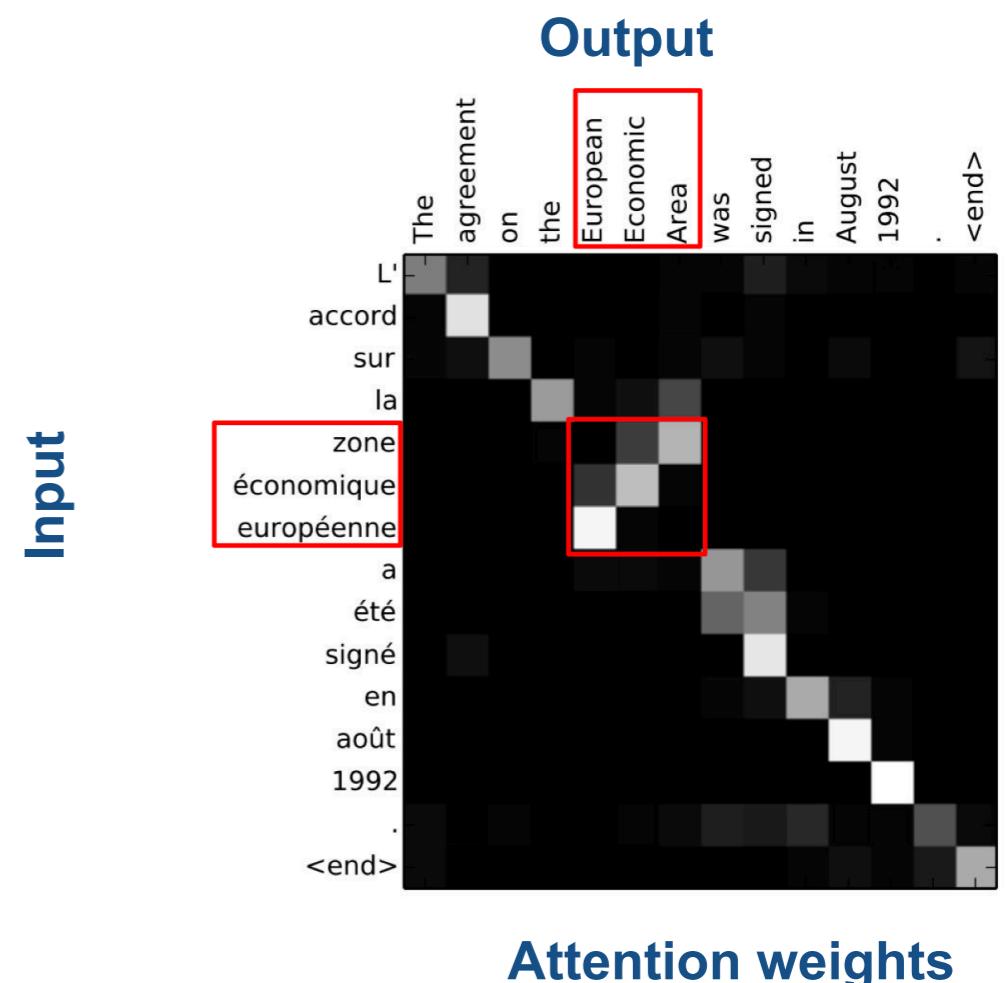
$$h_i^{l+1} = \text{MLP}^{l+1}\left((1 + \epsilon^l)h_i^l + \sum_{j \in \mathcal{N}_i} h_j^l\right)$$

$$h_{\mathcal{G}} = \text{MLP}\left(\sum_{i \in \mathcal{V}} h_i^{l_{max}}\right)$$

[Xu et al., How powerful are graph neural networks, ICLR 2019]

Attention mechanisms on graphs

- Attention is a mechanism through which neural networks dynamically allocate weights to distinct input based on their relevance
- It has shown to be key in tasks such as machine translation and language understanding



How can we extend attention to graph nodes?

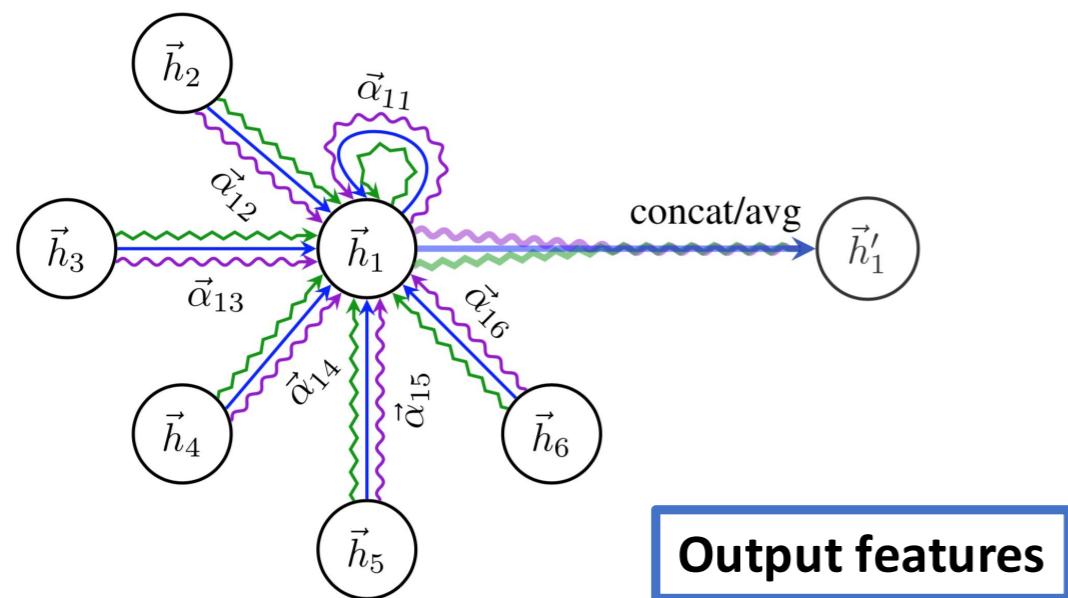
[Bahdanau et al, “Neural machine translation by jointly learning to align and translate”, ICLR 2015]

Graph attention networks (GAT)

- Previous message passing GNNs use fixed weights for incoming information

$$h_i^{l+1} = \sigma(\theta_0^l h_i^l + \sum_{j \in \mathcal{N}_i} \theta_1^l h_j^l)$$

- In attentional GNNs, weights depend on the neighbourhood's features
 - Different weights to different nodes in a neighbourhood
 - Remove dependence on the global graph structure



Updated embedding

$$h_i^{l+1} = \sigma(\alpha_{ii}^l \theta_0^l h_i^l + \sum_{j \in \mathcal{N}_i} \alpha_{ij}^l \theta_1^l h_j^l)$$

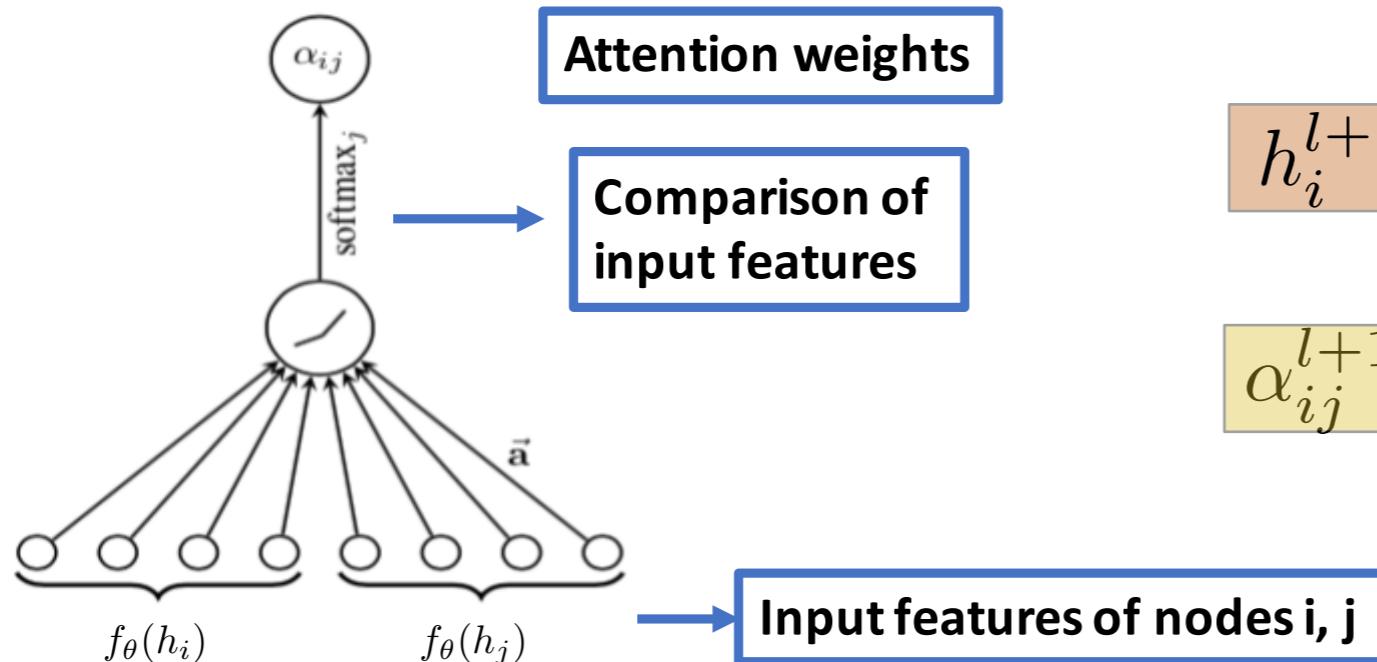
[Velickovic et al., Graph Attention Networks, ICLR 2018]

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- In attentional GNNs, weights depend on the neighbourhood's features
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$$h_i^{l+1} = \sigma(\alpha_{ii}^l \theta_0^l h_i^l + \sum_{j \in \mathcal{N}_i} \alpha_{ij}^l \theta_1^l h_j^l)$$
$$\alpha_{ij}^{l+1} = \alpha(f_\theta(h_i^{l+1}), f_\theta(h_j^{l+1}))$$

Updated edge attention

[Velickovic et al., Graph Attention Networks, ICLR 2018]

Summary of spatial methods

- **Pros:**

- Intuitive
- Easy to implement
- Generalize to inductive settings

- **Cons:**

- Lack of interpretation in the spectral domain
- Require many message passing iterations if the size of the graph is large

Useful resources

- **Toolboxes**
 - https://github.com/rusty1s/pytorch_geometric
 - <https://github.com/dmlc/dgl>
 - <https://github.com/deepmind/jraph>
 - <https://github.com/tensorflow/gnn>
- **Datasets**
 - DGL datasets: <https://docs.dgl.ai/api/python/dgl.data.html>
 - PyG datasets: <https://pytorch-geometric.readthedocs.io/en/latest/modules/datasets.html>
 - OGB datasets: <https://ogb.stanford.edu>
 - <https://chrsmrrs.github.io/datasets/>
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Summary

- Graph neural networks: A very active area of research
- Different architecture designs, most of them can be categorized as convolutional, message passing, attentional
- The expressive power of GNN architectures will be discussed in the next lecture!

References

1. Graph representation learning (chap 5), William Hamilton
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 - <https://arxiv.org/pdf/1812.08434.pdf>