Learning from Networks

Graph Neural Networks

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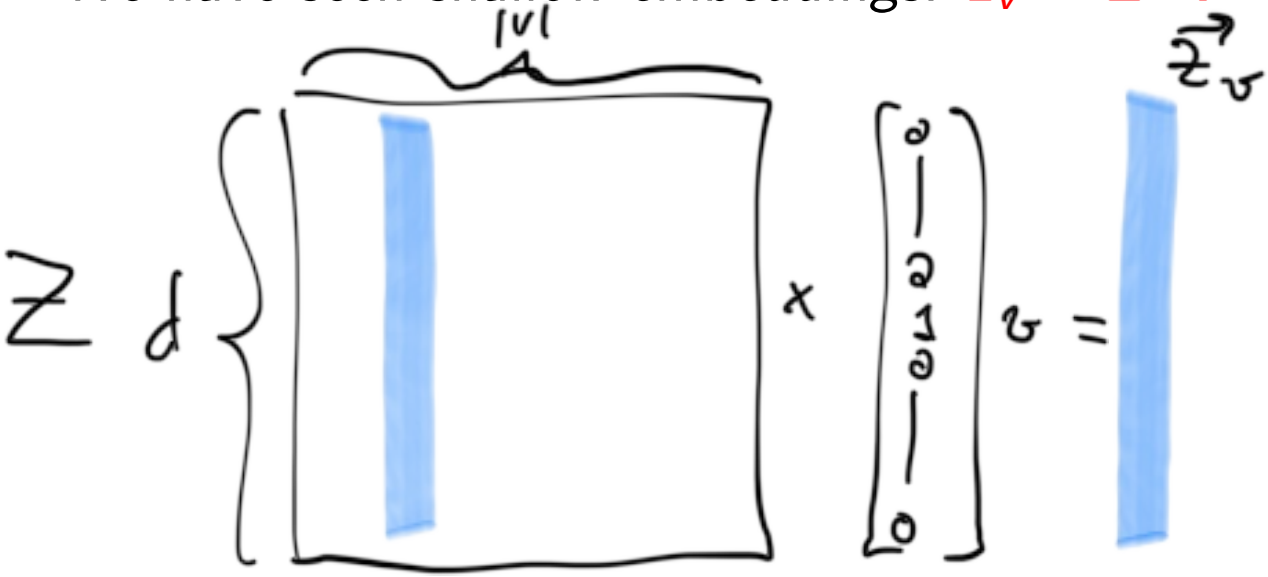
Shallow Embeddings

Node embedding task: given graph $G = (V, E)$, represent each $v \in V$ as $ENC(v) = \mathbf{z}_v \in \mathbb{R}^d$ such that similarities $S(u, v)$ in G are approximated by (decoded) similarities $DEC(\mathbf{z}_u, \mathbf{z}_v)$ for all $u, v \in V$:

$$S(u, v) \approx DEC(\mathbf{z}_u, \mathbf{z}_v)$$

We have seen *shallow embeddings*: $\mathbf{z}_v = \mathbf{Z} \cdot \mathbf{v}$



Shallow Embeddings: Limitations

Large number of parameters: high *complexity* of the *model*

Inherently *transductive*: cannot generate embeddings for nodes that are not present during the *training* phase

We would like *inductive* embedding methods: can generate the embeddings for new nodes

Do not incorporate node features: many networks have node features that can/should be used to produce the embedding

They are *unsupervised* methods: learned embeddings are independent of the (downstream) ML task

Graph Neural Network Embeddings: Main Idea

Instead of learning $\mathbf{z}_v$ for each $v \in V$, learn a function $f : V \to \mathbb{R}^d$

f is computed by a *neural network* that depends on the structure of the graph $\Rightarrow$ *graph neural network* (GNN)

Given the graph G and features of the nodes $v \in V$, the GNN can compute the embedding of *any* node $u \in V$

Encoder-decoder framework:

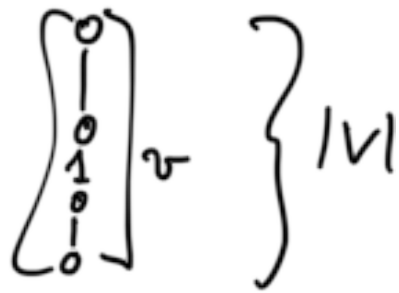
- the encoder $ENC()$ is a neural network
- other components (similarity, decoder, loss function): as for shallow embeddings

$\Rightarrow$ the parameters to be learned from the data are in the neural network

GNN: Setup

We have node features:

- social networks: user profile info, activity info, ...
- biological networks: gene expression profiles, functional information, ...
- what if no (external) features available?
  - compute node features: clustering coefficient, centrality scores, etc.
  - *one-hot encoding of a node* :



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  - *one-hot encoding of a node*
  - vector of all 1's

Given

- graph $G = (V, E)$, with $|V| = n$
- $\mathbf{A}$ is the adjacency matrix of G
- each node $v \in V$ has vector $\mathbf{x}_v \in \mathbb{R}^r$ of r *features*
- $\mathbf{X} \in \mathbb{R}^{r \times n}$ is the matrix of nodes features

Goal: we want to combine the features $\mathbf{x}_v$ of a node and the structural (topological) information from G to obtain encodings for each node $v \in V$

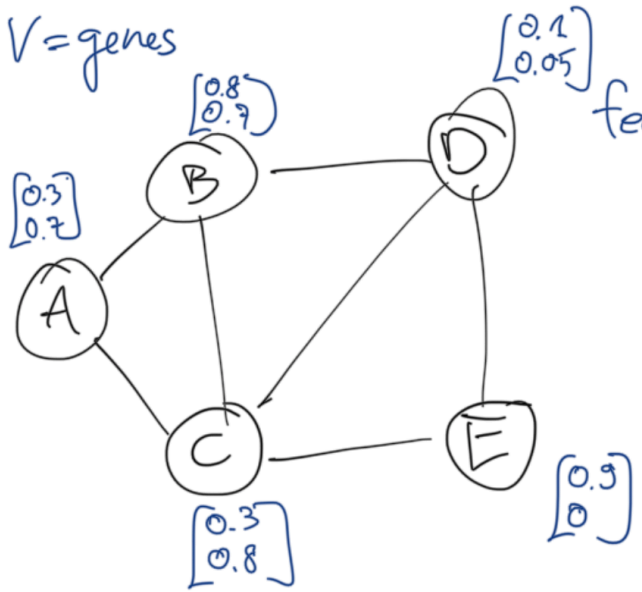
Ideas?

Naïve Approach

Idea:

- for each node $v \in V$, build an input vector that contains both the node features $\mathbf{x}_v$ and the *adjacency matrix vector* for v
- $ENC(v)$ is the output of a (deep) neural network whose input are the vectors above

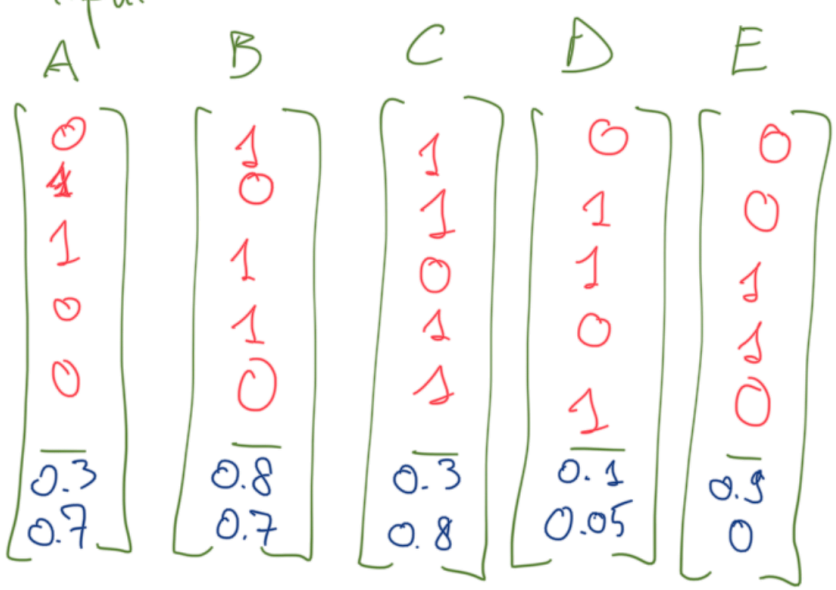
Example

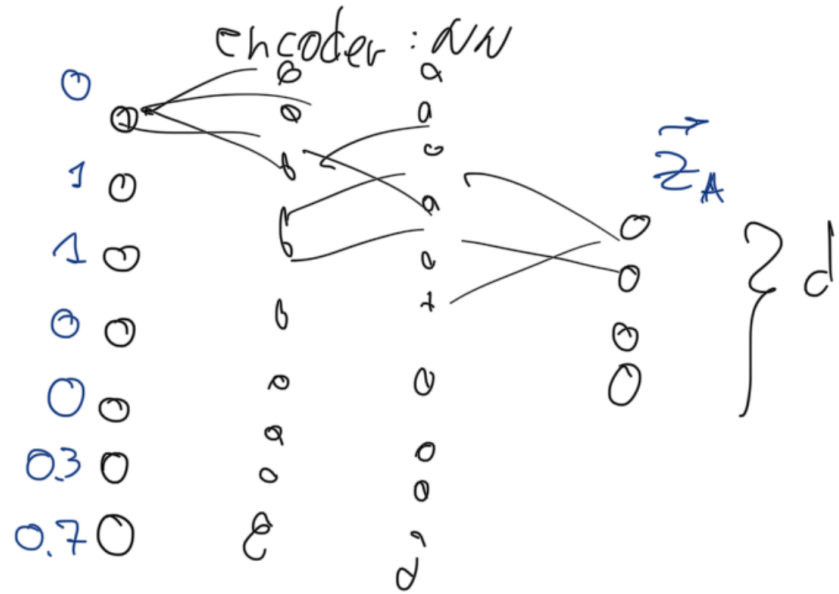


adjacency matrix:

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

input vectors for the NN:





Naïve Approach: Issues

Number of parameters? $\Omega(n)$ → because the input layer has $\Omega(n)$ nodes

Not applicable to graphs of different sizes → they have input layers of different sizes

Depends on the node ordering → if I change the order of nodes in the adjacency matrix, the embeddings of the nodes change

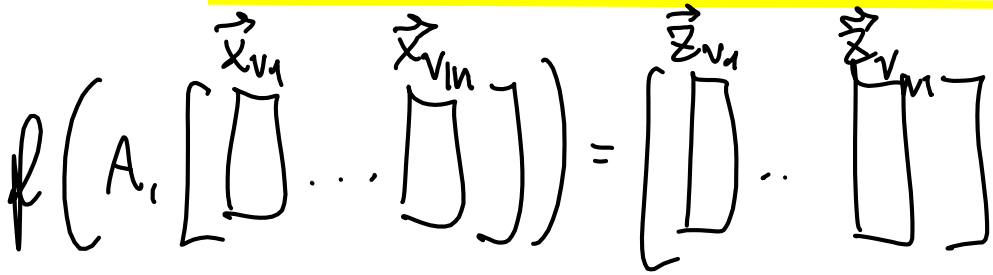
Permutation Invariance and Permutation Equivariance

We would like the embedding to be *independent* of the node ordering.

Let f be the function that given the adjacency matrix $\mathbf{A}$ of G and the feature matrix $\mathbf{X}$ of the nodes of G produces in output the embedding matrix $\mathbf{Z}$:

$$\mathbf{Z} = f(\mathbf{A}, \mathbf{X})$$

We would like f to be *permutation invariant* or *permutation equivariant*



Permutation Invariance and Permutation Equivariance (continue)

We would like it to be *permutation invariant* or *permutation equivariant*

Permutation matrix P: each row/column has exactly one 1, all other entries are 0.

Definition

f is *permutation invariant* if $f(\mathbf{PAP}^T, \mathbf{XP}^T) = f(\mathbf{A}, \mathbf{X})$ where $\mathbf{P}$ is a *permutation matrix*.

non originali, ma permutate

Definition

f is *permutation equivariant* if $f(\mathbf{PAP}^T, \mathbf{XP}^T) = f(\mathbf{A}, \mathbf{X})\mathbf{P}^T$ where $\mathbf{P}$ is a *permutation matrix*.

$\vec{P}\vec{A}$: permutare righe, $(\vec{P}\vec{A})\vec{P}^T$: permutare colonne

Example

$\ell(A, X) = z$, $G: |V| = 3$, $d = 2$

$$Z = \underbrace{\left[\begin{array}{c|c|c} z_{11} & z_{12} & z_{13} \\ z_{21} & z_{22} & z_{23} \end{array}\right]}_{|V|} d, \qquad P = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

$$Z \cdot P^T = \left[\begin{array}{c|c|c} z_{11} & z_{12} & z_{13} \\ z_{21} & z_{22} & z_{23} \end{array}\right] \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}^T = \left[\begin{array}{c|c|c} z_{11} & z_{12} & z_{13} \\ z_{21} & z_{22} & z_{23} \end{array}\right] \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} =$$

$$= \left[\begin{array}{c|c|c} z_{13} & z_{11} & z_{12} \\ z_{23} & z_{21} & z_{22} \end{array}\right]$$

Neural Message Passing Framework

Idea

- the computation proceeds in iterations
- in iteration k, the (hidden) embedding $\mathbf{h}_v^{(k)}$ for node v is updated/computed according to the (hidden) embeddings of nodes $u \in \mathcal{N}(v)$ ⇒ solo nodi vicini, non tutti
- the output embedding for node v is the embedding $\mathbf{h}_v^{(K)}$ after K iterations
- initialization: $\mathbf{h}_v^{(0)} = \mathbf{x}_v$ for all $v \in V$

Formally:

- $\texttt{AGGREGATE}^{(k)}\left(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\}\right) = \mathbf{m}_{\mathcal{N}(u)}^{(k)}$: function that given the (hidden) embeddings of neighbours of u at iteration k produces the *message* $\mathbf{m}_{\mathcal{N}(u)}^{(k)}$.
- $\texttt{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)}\right)$

$\texttt{AGGREGATE}^{(k)}(\dots)$ and $\texttt{UPDATE}^{(k)}(\dots)$ are arbitrarily differentiable functions ⇒ neural networks ⇒ implementate con NN semplici

Neural Message Passing Framework

Then for each $u \in V$:

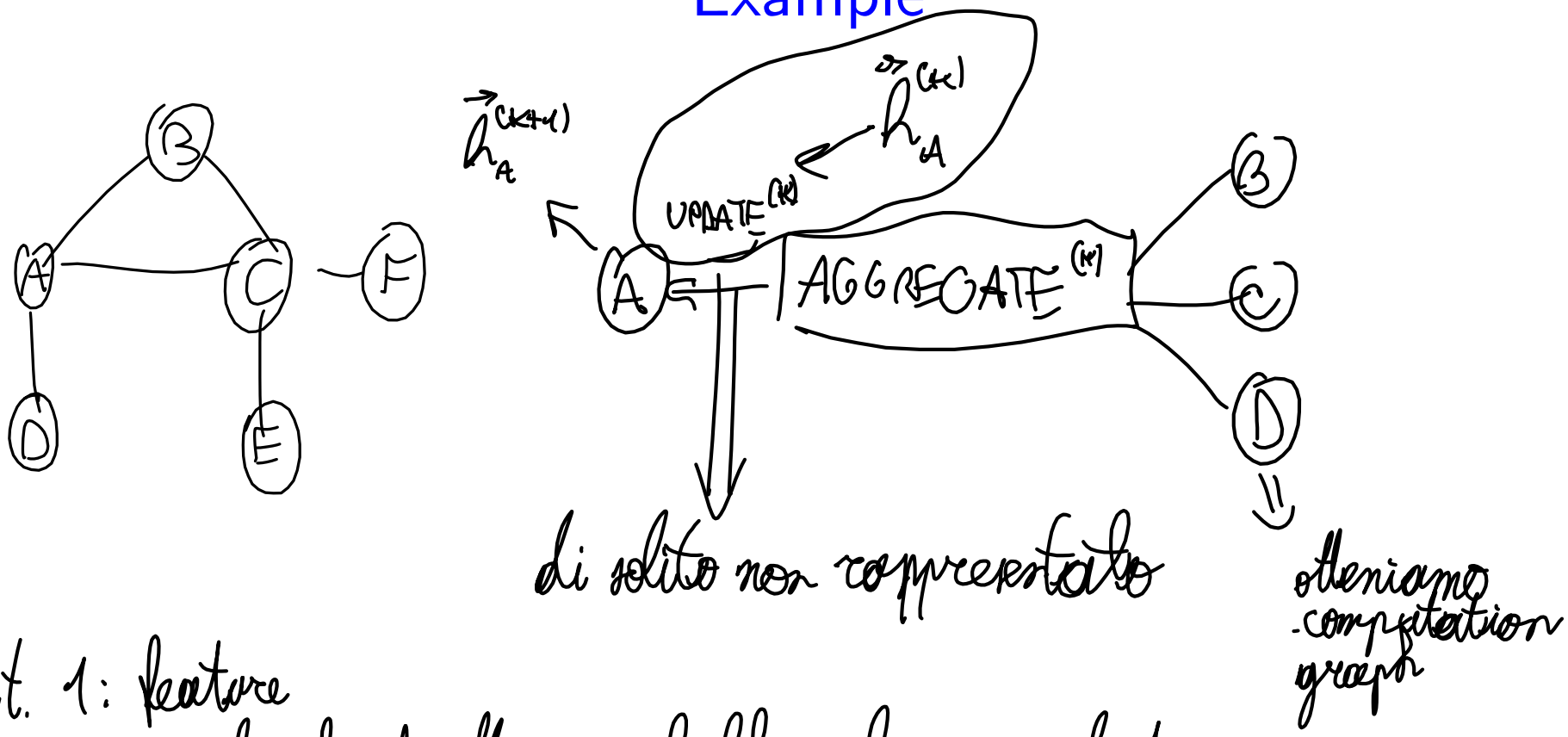
$$\mathbf{h}_u^{(k+1)} = \texttt{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \texttt{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\})\right)$$
$$= \texttt{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)}\right)$$

The embedding $\mathbf{z}_u$ of a node $u \in V$ is the embedding after K iterations:

$$\mathbf{z}_u = \mathbf{h}_u^{(K)}$$

Note: the iterations of message passing are also called *layers* of the GNN

Example



di solito non rappresentato

otteniamo computation graph

it. 1: feature

// 2: guardando A, ottengo embedding dei vicini di A e rappr. di A da it. 1

funzioni sempre uguali all'interno di it., possono essere diverse per it. diverse

con K it., $\vec{h}_v^{(K)}$ dipende da feature di nodi a distanza $\leq K$

Example

computation graph diverso $\forall$ nodo, ma UPDATE e AGGREGATE condivise da tutti nodi

In generale, comp. graph = NNs con parametri condivisi $\Rightarrow$ riduce # parametri $\Rightarrow$ riduce complessità modello

Example

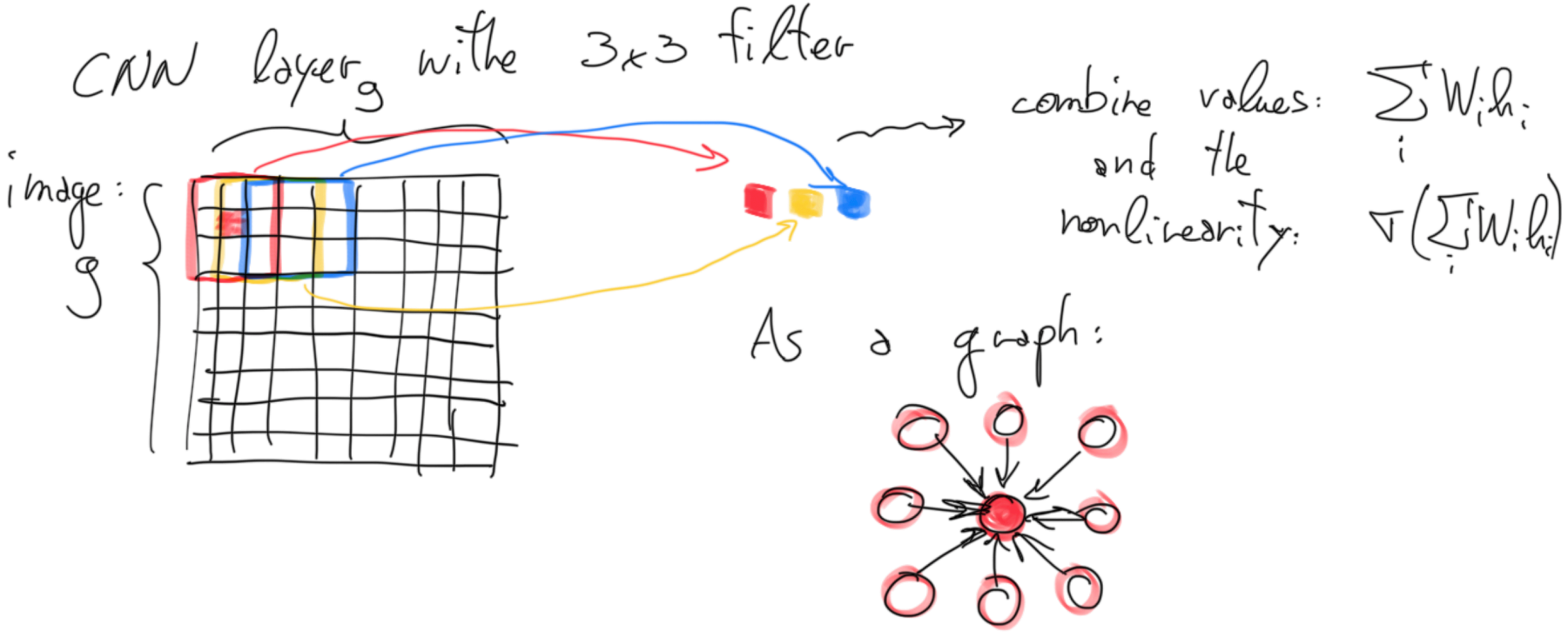
Neural Message Passing Framework

Question: are GNNs (as generally defined in the previous slide) sensible to permutations of the nodes?

The `AGGREGATE` function works on sets, so if we consider "proper" `AGGREGATE` functions (i.e., the order of the input elements does not matter) and "proper" `UPDATE` functions $\Rightarrow$ the resulting GNN is permutation invariant

Neural Message Passing: Motivation

Intuition: the local feature-aggregation behaviour of GNNs is analogous to the behavior of the convolutional filters in CNNs



Basic GNNs

The most basic version of a GNN is given by:

$$\texttt{AGGREGATE}^{(k)}\left(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\}\right) = \mathbf{m}_{\mathcal{N}(u)}^{(k)} = \sum_{v \in \mathcal{N}(u)} \mathbf{h}_v^{(k)}$$

Therefore:

$$\begin{aligned}\mathbf{h}_u^{(k+1)} &= \texttt{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)}\right) \\ &= \sigma\left(\mathbf{W}_{\text{self}}^{(k+1)}\mathbf{h}_u^{(k)} + \mathbf{W}_{\text{neigh}}^{(k+1)}\mathbf{m}_{\mathcal{N}(u)}^{(k)} + \mathbf{b}^{(k+1)}\right)\end{aligned}$$

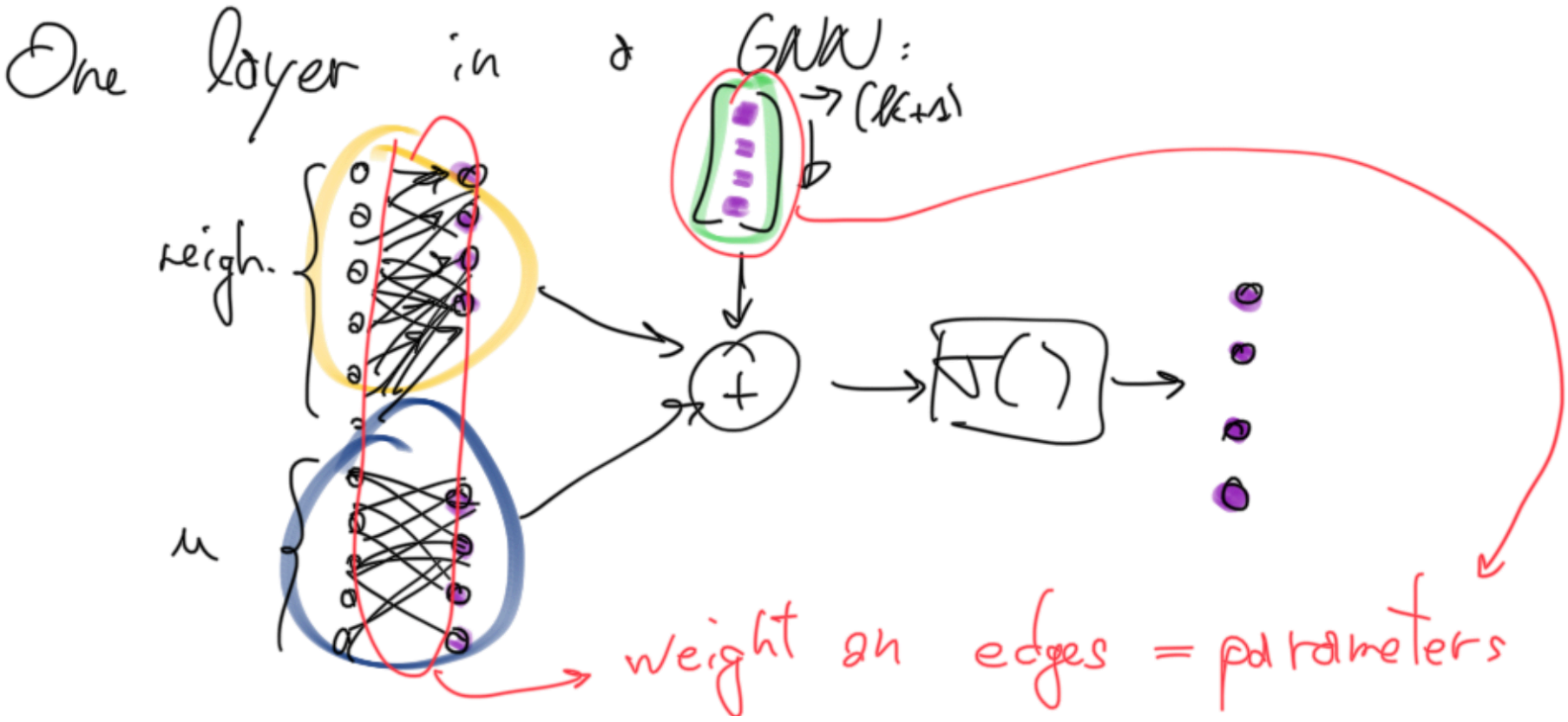
Notes

- $\mathbf{W}_{\text{self}}^{(k+1)}$ and $\mathbf{W}_{\text{neigh}}^{(k+1)}$ are trainable parameters, with $\mathbf{W}_{\text{self}}^{(k+1)}, \mathbf{W}_{\text{neigh}}^{(k+1)} \in \mathbb{R}^{d^{(k+1)} \times d^{(k)}}$
- $\mathbf{b}^{(k+1)}$ is the *bias*; often omitted in the notation
- $\sigma()$ is an *elementwise* non-linear function (e.g., ReLU)

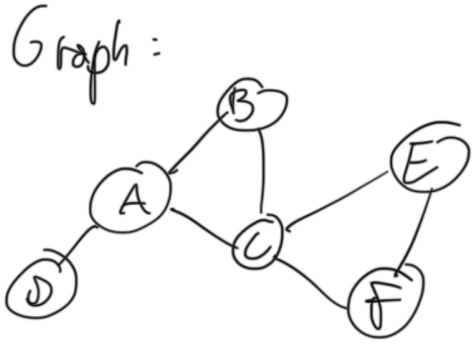
Basic GNNs (continue)

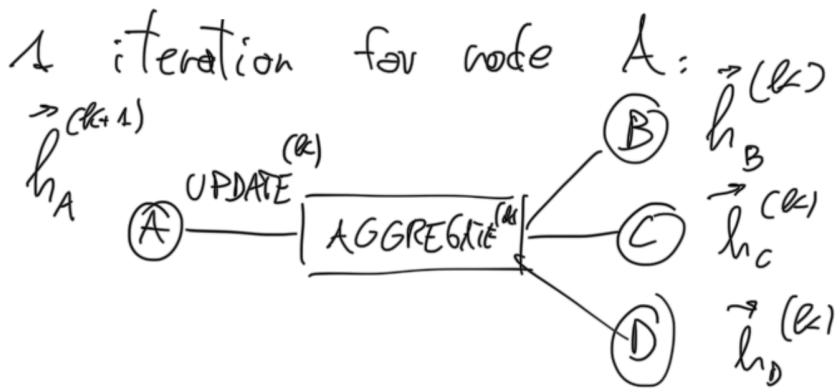
Putting all together, for each node u, in each iteration:

$$\mathbf{h}_u^{(k+1)} = \sigma\left(\mathbf{W}_{\text{self}}^{(k+1)}\mathbf{h}_u^{(k)} + \mathbf{W}_{\text{neigh}}^{(k+1)} \sum_{v \in \mathcal{N}(u)} \mathbf{h}_v^{(k)} + \mathbf{b}^{(k+1)}\right)$$



Example



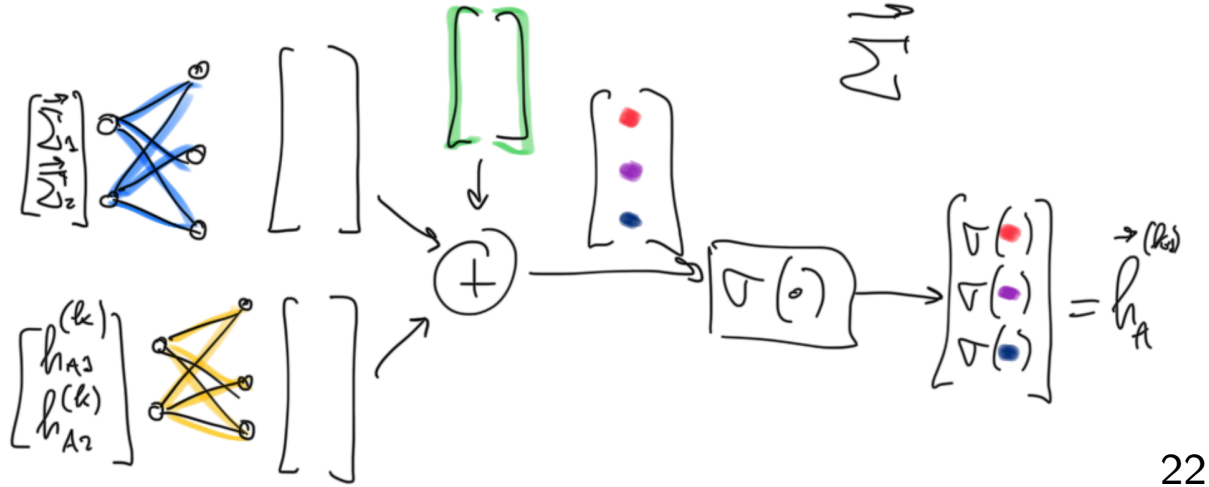


$$d^{(k)} = 2$$

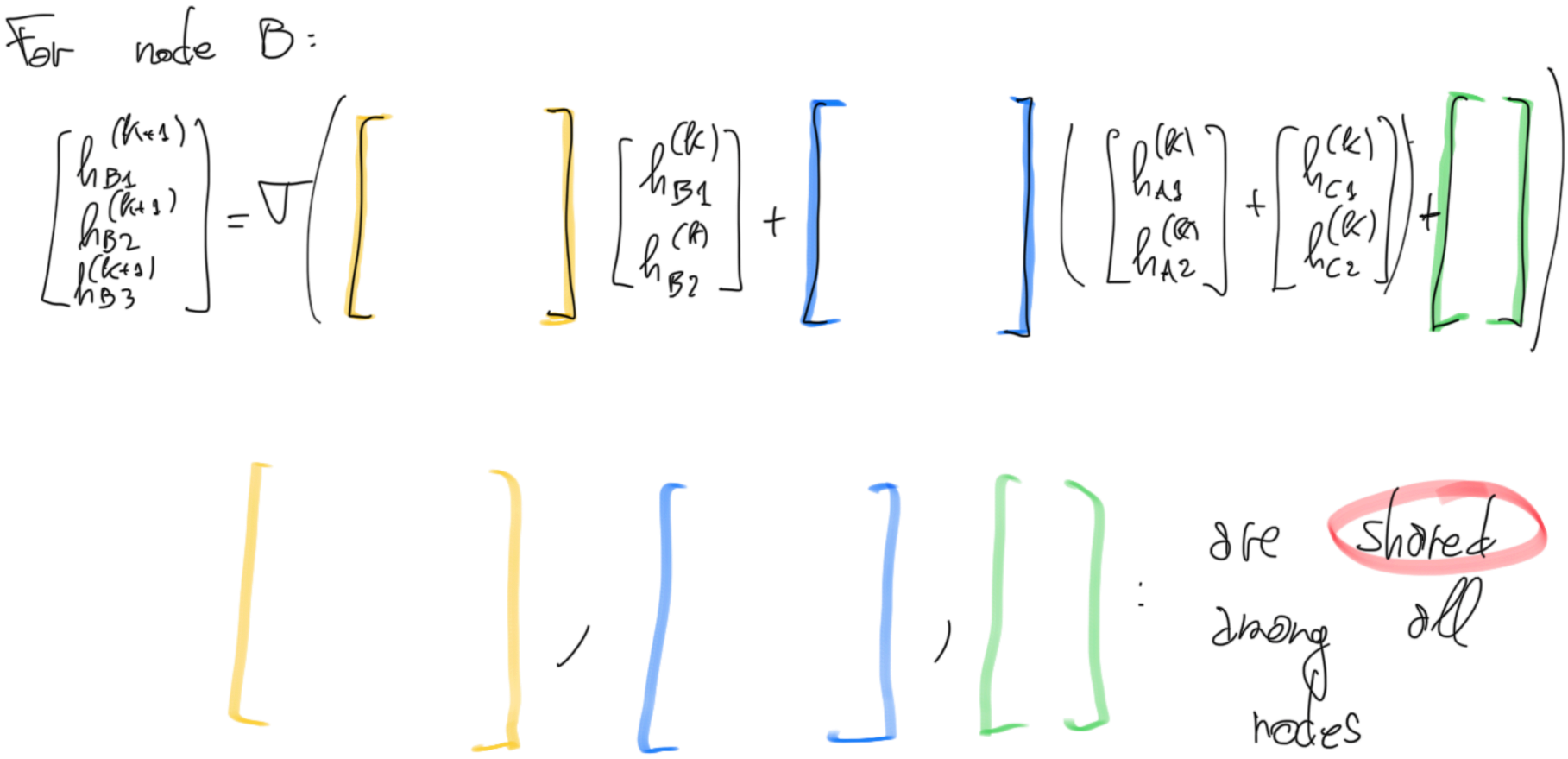
$$d^{(k+1)} = 3$$

$$\begin{bmatrix} h_{A1}^{(k+1)} \\ h_{A2}^{(k+1)} \\ h_{A3}^{(k+1)} \end{bmatrix} = \sigma\left(\begin{bmatrix} W_{s11} & W_{s12} \\ W_{s21} & W_{s22} \\ W_{s31} & W_{s32} \end{bmatrix} \begin{bmatrix} h_{A1}^{(k)} \\ h_{A2}^{(k)} \end{bmatrix} + \begin{bmatrix} W_{n11} & W_{n12} \\ W_{n21} & W_{n22} \\ W_{n31} & W_{n32} \end{bmatrix} \left(\begin{bmatrix} h_{B1}^{(k)} \\ h_{B2}^{(k)} \end{bmatrix} + \begin{bmatrix} h_{C1}^{(k)} \\ h_{C2}^{(k)} \end{bmatrix} + \begin{bmatrix} h_{D1}^{(k)} \\ h_{D2}^{(k)} \end{bmatrix} \right) + \begin{bmatrix} b_1^{(k+1)} \\ b_2^{(k+1)} \\ b_3^{(k+1)} \end{bmatrix} \right)$$

Σ



Example



Basic GNNs: Parameter Sharing

The neural networks in different iterations can share parameters

$\mathbf{W}_{\text{self}}^{(k+1)}$, $\mathbf{W}_{\text{neigh}}^{(k+1)}$, $\mathbf{b}^{(k+1)}$ can be shared across the GNN iterations (layers).

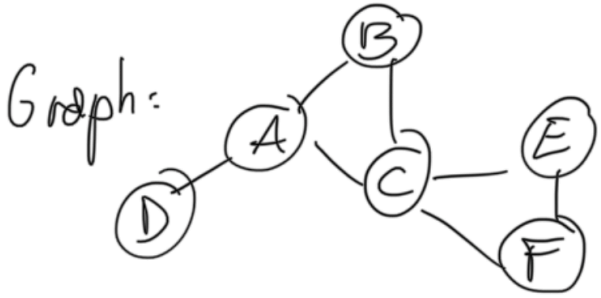
That is $\mathbf{W}_{\text{self}}^{(k+1)} = \mathbf{W}_{\text{self}}$, $\mathbf{W}_{\text{neigh}}^{(k+1)} = \mathbf{W}_{\text{neigh}}$ and $\mathbf{b}^{(k+1)} = \mathbf{b}$ for all $k \in \{0, \ldots, K-1\}$

In this case:

$$\mathbf{h}_u^{(k+1)} = \sigma\left(\mathbf{W}_{\text{self}}\mathbf{h}_u^{(k)} + \mathbf{W}_{\text{neigh}} \sum_{v \in \mathcal{N}(u)} \mathbf{h}_v^{(k)} + \mathbf{b}\right)$$

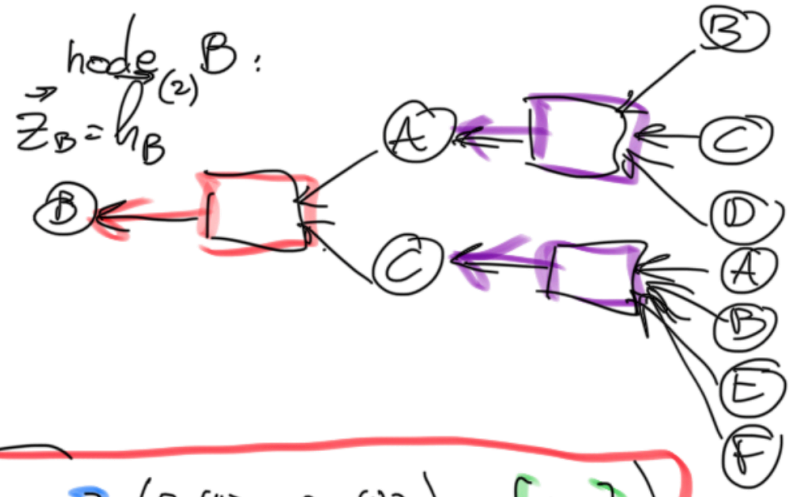
Note: this implies that $d^{(k)} = d \quad \forall k = 1, \ldots, K$

Example



$K = 2$

$d = 3$



$$\begin{bmatrix} h_{B1}^{(2)} \\ h_{B2}^{(2)} \\ h_{B3}^{(2)} \end{bmatrix} = \sigma\left(\begin{bmatrix} W_{S11} & W_{S12} & W_{S13} \\ W_{S21} & W_{S22} & W_{S23} \\ W_{S31} & W_{S32} & W_{S33} \end{bmatrix} \begin{bmatrix} h_{B1}^{(1)} \\ h_{B2}^{(1)} \\ h_{B3}^{(1)} \end{bmatrix} + \overbrace{\left[\quad \right]}^{3} \left(\begin{bmatrix} h_{A1}^{(1)} \\ h_{A2}^{(1)} \\ h_{A3}^{(1)} \end{bmatrix} + \begin{bmatrix} h_{C1}^{(1)} \\ h_{C2}^{(1)} \\ h_{C3}^{(1)} \end{bmatrix} \right) + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

$$\begin{bmatrix} h_{A1}^{(1)} \\ h_{A2}^{(1)} \\ h_{A3}^{(1)} \end{bmatrix} = \sigma\left(\begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \begin{bmatrix} h_{A1}^{(0)} \\ h_{A2}^{(0)} \\ h_{A3}^{(0)} \end{bmatrix} + \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \left(\vec{h}_B^{(0)} + \vec{h}_C^{(0)} + \vec{h}_D^{(0)} \right) + \begin{bmatrix} \\ \\ \end{bmatrix} \right)$$

Graph-Level Equations

Many GNNs can be succinctly defined using *graph-level* equations.

For the basic GNN, they are:

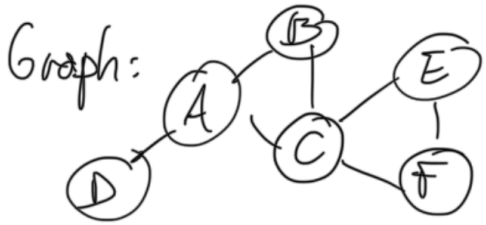
$$\mathbf{H}^{(k)} = \sigma\left(\mathbf{A}\mathbf{H}^{k-1}\mathbf{W}_{\text{neigh}} + \mathbf{H}^{k-1}\mathbf{W}_{\text{self}} + \mathbf{B}\right)$$

where:

- $\mathbf{A}$ is the adjacency matrix of G
- $\mathbf{H}^k \in \mathbb{R}^{|V| \times d^{(k)}}$ is the matrix of node representations at layer k of the GNN: each row is the representation of a node at layer k
- $\mathbf{B} \in \mathbb{R}^{|V| \times d^{(k)}}$ is the *bias* matrix, where each row is equal to the bias vector $\mathbf{b}$

Note: the GNN can be efficiently implemented with a small number of *sparse* matrix operations.

Example



$$H^{(k)} = \begin{bmatrix} \vec{h}_A^{(k)} \\ \vec{h}_B^{(k)} \\ \vec{h}_C^{(k)} \\ \vec{h}_D^{(k)} \\ \vec{h}_E^{(k)} \\ \vec{h}_F^{(k)} \end{bmatrix} = \sigma\left(\begin{array}{c} \begin{array}{cccccc} A & B & C & D & E & F \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix} \end{array} \begin{bmatrix} \vec{h}_A^{(k-1)} \\ \vec{h}_B^{(k-1)} \\ \vec{h}_C^{(k-1)} \\ \vec{h}_D^{(k-1)} \\ \vec{h}_E^{(k-1)} \\ \vec{h}_F^{(k-1)} \end{bmatrix} \begin{bmatrix} W_{neigh} \end{bmatrix} + \right.$$

$$\left. + \begin{bmatrix} \vec{h}_A^{(k-1)} \\ \vec{h}_B^{(k-1)} \\ \vec{h}_C^{(k-1)} \\ \vec{h}_D^{(k-1)} \\ \vec{h}_E^{(k-1)} \\ \vec{h}_F^{(k-1)} \end{bmatrix} \begin{bmatrix} W_{self} \end{bmatrix} + \begin{bmatrix} \vec{b} \\ \vec{b} \\ \vec{b} \\ \vec{b} \\ \vec{b} \\ \vec{b} \end{bmatrix} \right)$$

first row

$$\begin{bmatrix} \vec{h}_A^{(k)} \end{bmatrix} = \sigma\left(\begin{bmatrix} \vec{h}_B^{(k-1)} + \vec{h}_C^{(k-1)} + \vec{h}_D^{(k-1)} \end{bmatrix} \begin{bmatrix} W_{neigh} \end{bmatrix} + \begin{bmatrix} \vec{h}_A^{(k-1)} \end{bmatrix} \begin{bmatrix} W_{self} \end{bmatrix} + \begin{bmatrix} \vec{b} \end{bmatrix} \right)$$

Message Passing with Self-loops

Simplification of neural message passing: omit the *update* operator by adding self loops to the graph.

With this modification, each iteration of a general GNN is:

$$\mathbf{h}_u^{(k+1)} = \texttt{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u) \cup \{u\}\})$$

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This is a simplification of a general GNN

- pro: reduces overfitting
- con: limits the *expressivity* of the GNN

Message Passing with Self-loops (continue)

For the basic GNN: adding self-loops means sharing parameters between $\mathbf{W}_{\text{self}}$, $\mathbf{W}_{\text{neigh}}$, that is:

$$\mathbf{W}_{\text{self}} = \mathbf{W}_{\text{neigh}} = \mathbf{W}$$

Example

Generalized Neighborhood Aggregation

The basic GNN can be improved and generalized in several ways.

We now see how to generalize the AGGREGATE operator.

For each $u \in V$:

$$\mathbf{h}_u^{(k+1)} = \texttt{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \texttt{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\})\right)$$
$$= \texttt{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)}\right)$$

Neighborhood Normalization

Issue of Basic GNN: it is sensitive to node degrees.

Neighborhood Normalization

Issue of Basic GNN: it is sensitive to node degrees.

Solution: normalize the `AGGREGATE` operator taking into account the degree.

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

Better solution in practice:

$$\mathbf{m}_{\mathcal{N}(u)}^{(k)} = \sum_{v \in \mathcal{N}(u)} \frac{\mathbf{h}_v^{(k)}}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}}$$

Graph convolutional networks (GCNs)

Introduced by Kipf and Welling, *Semi-supervised classification with graph convolutional networks*, ICLR 2016.

Uses the neighborhood normalization with self-loops.

For each $u \in V$:

GraphSAGE

Introduced by W.L. Hamilton, R. Ying, and J. Leskovec. *Inductive representation learning on large graphs*, NeurIPS (2017).

Introduced the generalized aggregation AGGREGATE operator.

Main differences with GCNs:

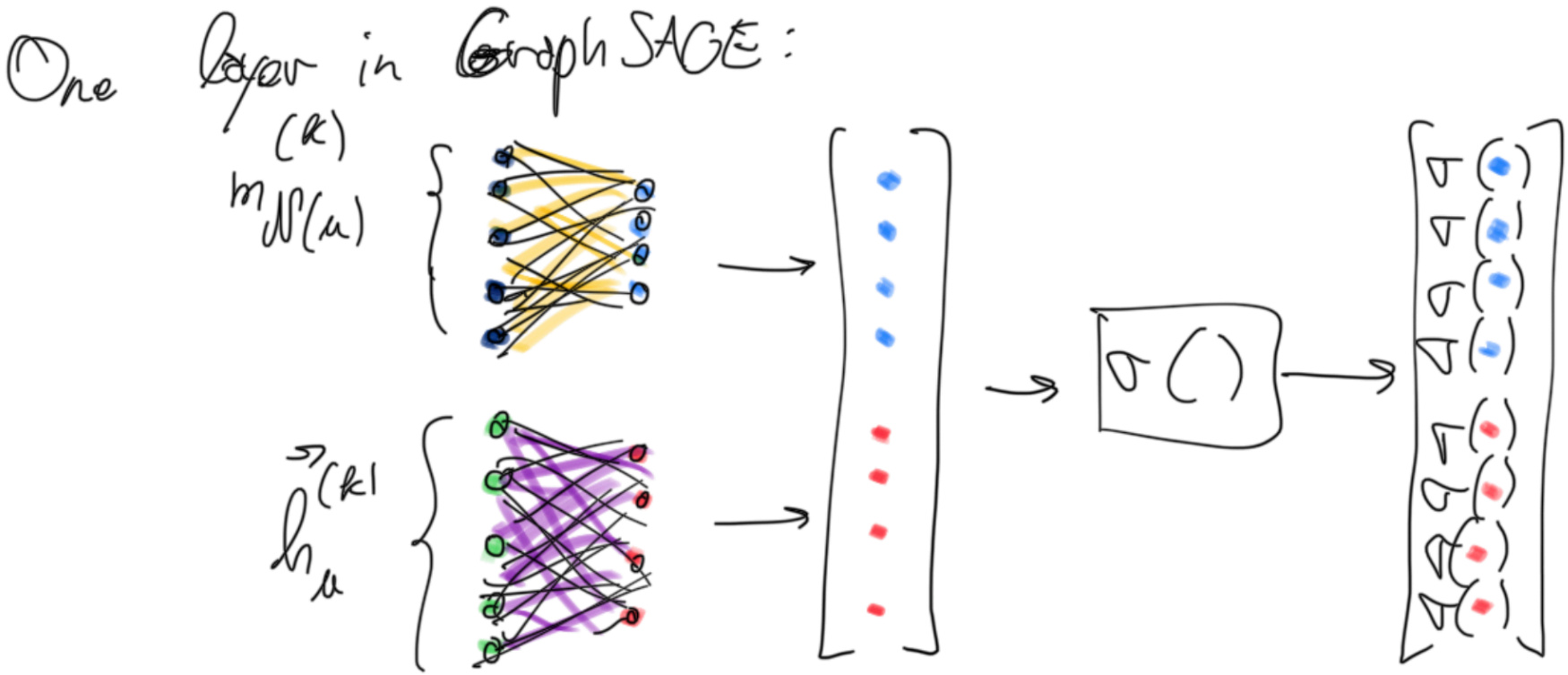
- use of generalized AGGREGATE operator
- for each node u, a transformation of $\mathbf{h}_u^{(k)}$ is *concatenated* with the transformation of $\mathbf{m}_{\mathcal{N}(u)}^{(k)}$ (before the elementwise nonlinear operator is applied)

GraphSAGE (continue)

For each node $u \in V$:

$$\mathbf{h}_u^{(k+1)} = \sigma\left(\left[\mathbf{W}^{(k+1)}\mathbf{m}_{\mathcal{N}(u)}^{(k)}, \mathbf{B}^{(k+1)}\mathbf{h}_u^{(k)}\right]\right)$$

where $\mathbf{m}_{\mathcal{N}(u)}^{(k)} = \texttt{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u) \cup \{u\}\})$



GraphSAGE (continue)

For each node $u \in V$:

$$\mathbf{h}_u^{(k+1)} = \sigma\left(\left[\mathbf{W}^{(k+1)}\mathbf{m}_{\mathcal{N}(u)}^{(k)}, \mathbf{B}^{(k+1)}\mathbf{h}_u^{(k)}\right]\right)$$

where $\mathbf{m}_{\mathcal{N}(u)}^{(k)} = \texttt{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u) \cup \{u\}\})$

Common choices for `AGGREGATE`:

- mean of $\mathbf{h}_v^{(k)}$:

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

- first apply a simple NN to each $\mathbf{h}_v^{(k)}$ (with learnable parameters θ), and then apply an elementwise operator γ (e.g., mean/max):

$$\mathbf{m}_{\mathcal{N}(u)}^{(k)} = \gamma\left(\left\{NN_\theta(\mathbf{h}_v^{(k)}), \forall u \in V\right\}\right)$$

- more complex functions (e.g., LSTM)

Graph Attention Network (GAT)

Introduced by P. Velickovic, G. Cucurull, A. Casanova, A. Romero, P. Lio, and Y. Bengio. *Graph attention networks*, ICLR (2018).

Neighborhood attention: assign an *attention* weight to each neighbor, which is used to weigh this neighbor's influence during aggregation

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

$\alpha_{u,v}$: attention on node $v \in \mathcal{N}(u)$ when aggregating information at node u

The attention weights $\alpha_{u,v}$ are learned from data.

GAT: Attention Weights

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

Various definitions of $\alpha_{u,v}$ have been used. The original one is:

$$\alpha_{u,v} = \frac{e^{\mathbf{a}^T [\mathbf{W}\mathbf{h}_u^{(k)}, \mathbf{W}\mathbf{h}_v^{(k)}]}}{\sum_{v \in \mathcal{N}(u)} e^{\mathbf{a}^T [\mathbf{W}\mathbf{h}_u^{(k)}, \mathbf{W}\mathbf{h}_v^{(k)}]}}$$

with

- $[\mathbf{W}\mathbf{h}_u^{(k)}, \mathbf{W}\mathbf{h}_v^{(k)}]$: concatenation of $\mathbf{W}\mathbf{h}_u^{(k)}$ and $\mathbf{W}\mathbf{h}_v^{(k)}$
- $\mathbf{W}$ is a matrix of parameters
- $\mathbf{a}^T$ is an *attention* vector

Generalized Update Operators

The UPDATE operator can be generalized as well (see the book if interested).
Why is this useful?

K. Xu, et al. *Representation learning on graphs with jumping knowledge networks*, ICML (2018) proved a result about *over-smoothing*, which we describe with the informal version below,

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Xu et al. consider *GCN-style networks*:

- AGGREGATE is essentially the mean
- UPDATE is done with self-loops

Informal version: when using a GCN-style network with K layers, the *influence* of node u on node v is proportional the probability $\Pr_k[v|u]$ of reaching node v on a random walk with K steps starting from node u.

GNNs: Graph Level

What about using GNNs to learn the embedding $\mathbf{z}_G$ of a graph G?

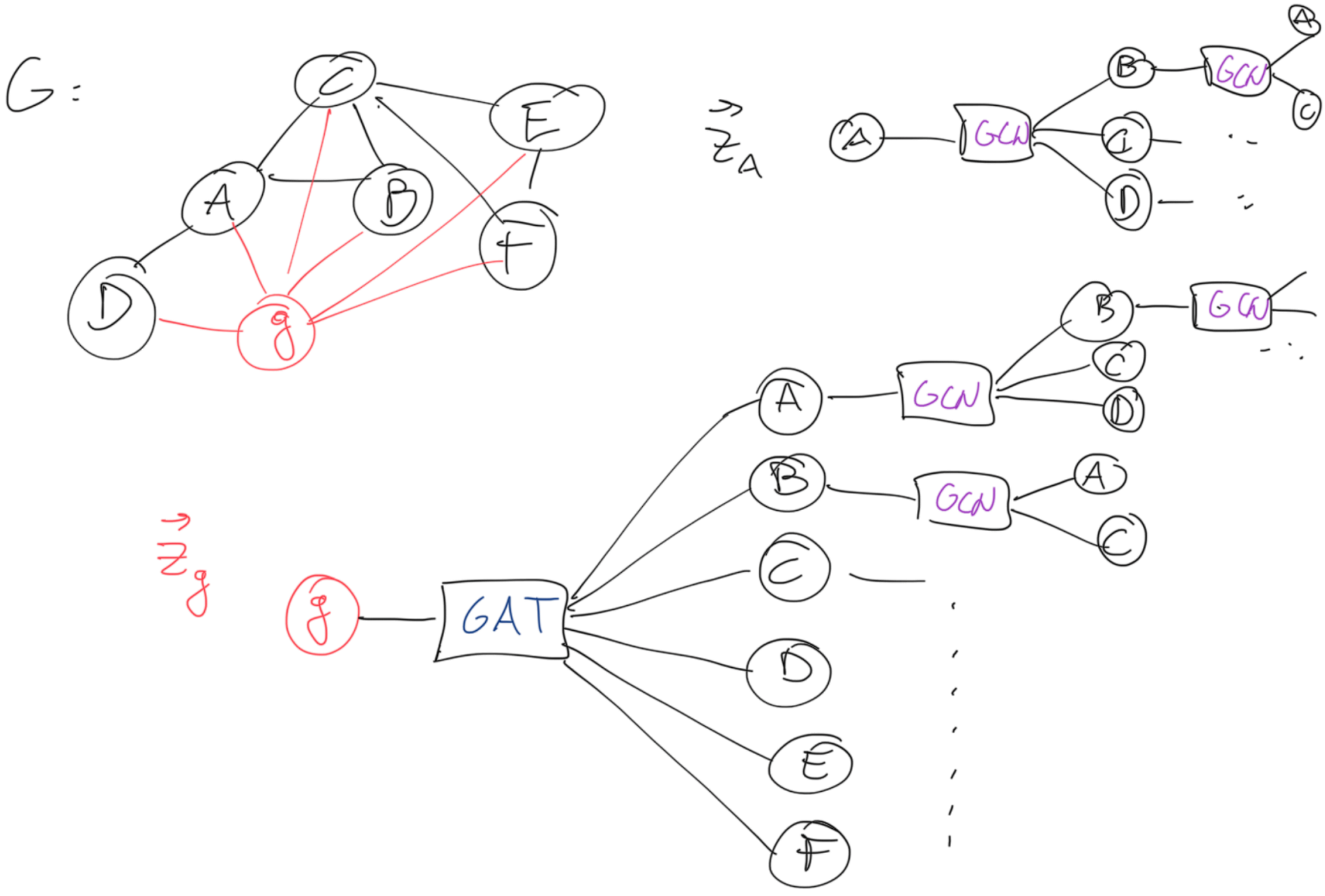
Approaches seen for graph embeddings usually work well, at least for small graphs:

- $\mathbf{z}_G = \sum_{u \in V} \mathbf{z}_u$
- add a node g connected to all $u \in V$, then $\mathbf{z}_G = \mathbf{z}_g$

More complex approaches recently explored (e.g., use LSTM).

Note: the second approach above can be made more flexible by using a specific neural network for g

GNNs: Graph Level (continue)

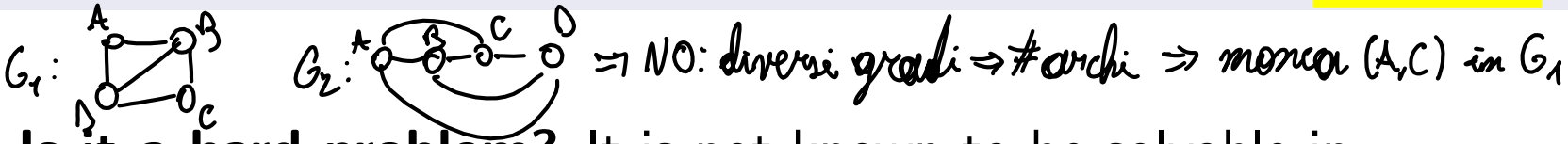


GNNs: a Theoretical Motivation

We will now see a theoretical motivation for GNNs, by comparing them with an algorithm for the *graph isomorphism problem*.

Definition

Given two graphs G_1 and G_2, the *graph isomorphism problem* requires to determine whether G_1 is isomorphic to G_2: $G_1 \simeq G_2$



Is it a hard problem? It is not known to be solvable in polynomial time nor to be NP-complete.

Note: ideally we would like a graph embedding technique to *solve* the graph isomorphism problem, that is: $\mathbf{z}_{G_1} = \mathbf{z}_{G_2}$ if and only if $G_1 \simeq G_2$

Weisfieler-Leman (WL) Algorithm

Algorithm for the graph isomorphism problem.

Note: does not always produce the correct answer!

- if WL outputs that $G_1 \not\simeq G_2$ then $G_1 \not\simeq G_2$
- if WL outputs that $G_1 \simeq G_2$, then it may be that $G_1 \not\simeq G_2$

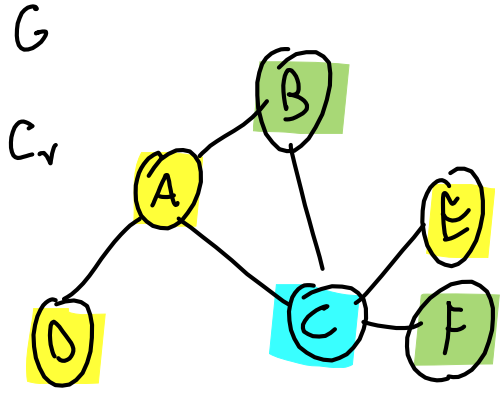
It is known that WL produces the correct answer for a large class of graphs.

WL Algorithm

Builds on a *color* refinement algorithm for the vertices of a graph G.

no random color

Given a coloring C_V of the vertices V of $G = (V, E)$, let $P(C_V)$ the partition of the vertices V defined by the coloring C_V: two vertices u, v are in the same set of the partition if and only if u and v have the same color.



$P(C_V) = \{A, D, E\}, \{C\}, \{B, F\}$

WL Algorithm (continue)

Algorithm `ColorRefinement`(G)
Input: graph $G = (V, E)$
Output: coloring of V

"color": hash value basato su hash values di vicini ⇒ calcolato efficientemente

$C_{curr} \leftarrow$ assign the same color u to all nodes $u \in V$;
repeat
  $C_{prev} \leftarrow C_{curr}$;
  $C_{curr} \leftarrow$ for each pair u and v where u and v have the same color in C_{prev}: assign different colors to u and v if and only if there is some color c such that u and v have different number of neighbours of color c in C_{prev};
until $P(C_{prev}) = P(C_{curr})$;
return C_{curr};

Analysis:

- `ColorRefinement`(G) stops after at most $|V|$ iterations;
- each iteration requires $O(|V|^2)$ operations
- the complexity of `ColorRefinement`(G) is $O(|V|^3)$

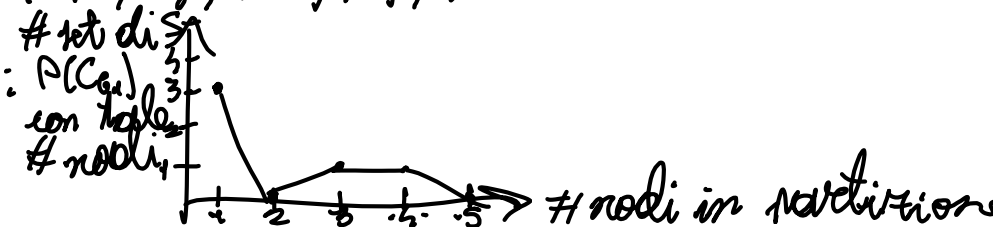
WL Algorithm (continue)

Algorithm $\texttt{WL}(G_1, G_2)$
Input: graphs $G_1 = (V_1, E_1)$, $G_2 = (V_2, E_2)$
Output: yes/no

$C_{G_1} \leftarrow \texttt{ColorRefinement}(G_1)$;
$C_{G_2} \leftarrow \texttt{ColorRefinement}(G_2)$;
return $\mathit{histogram}(P(C_{G_1})) = \mathit{histogram}(P(C_{G_2}))$;

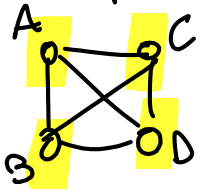
Analysis: the complexity of $\texttt{WL}(G_1, G_2)$ is $O\left(|V_1|^3 + |V_2|^3\right)$

G_1: $V = \{1, \ldots, 10\}$ ⇒ dopo colorRefinement(G_1), ho coloring C_{G_1} con
$P(C_{G_1}) = \{1, 3, 5, 10\}, \{7, 8, 9\}, \{2\}, \{4\}, \{6\}$ ⇒
⇒ histogram($P(C_{G_1})$):



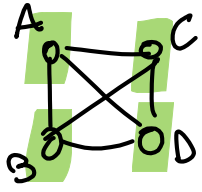
Example

Color refinement (G_1):

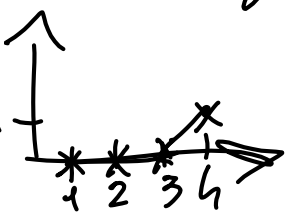


$P = \{A, B, C, D\}$

B: 3 vicini gialli, A: 3, C: 3, D: 3 $\Rightarrow$ coloring non cambia

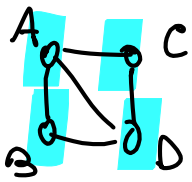


$P = \{A, B, C, D\} \Rightarrow C_{G_1}$:



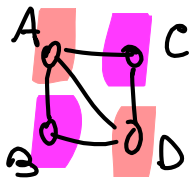
Example

ColorRefinement(G_2):



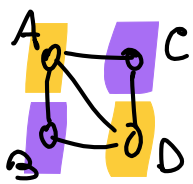
$P = \{A, B, C, D\} \Rightarrow$ A: 3 vicini blu, B: 2, C: 2, D: 3

it 2:

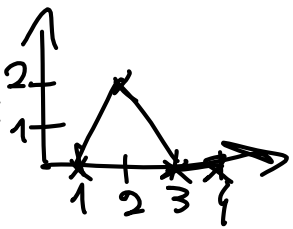


$P = \{A, D\}, \{B, C\} \Rightarrow$ A: 2,1 B: 0,2 C: 0,2 D: 2,1

it. 3:



$P = \{A, D\}, \{B, C\} \Rightarrow C_{G_2}$:



output: $G_1 \neq G_2 \Rightarrow$ sorretto

Example

WL "no" con $G_1 \simeq G_2$: impossibile

WL "yes" con $G_1 \not\simeq G_2$: possibile

WL algorithm and GNNs

Theorem

Consider a GNN with K message passing layers of the following form:

$$\mathbf{h}_u^{(k+1)} = \mathit{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathit{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\})\right)$$

where $\mathit{AGGREGATE}$ is differentiable and permutation invariant and UPDATE is differentiable. Assume that the input is made of discrete features: $\mathbf{h}_u^{(0)} = \mathbf{x}_u \in \mathbb{Z}^d, \forall u \in V$.
Then $\mathbf{h}_u^{(K)} \neq \mathbf{h}_v^{(K)}$ only if u and v have different labels after K iterations of the WL algorithm.

Informally: GNNs are *no more powerful than* the WL algorithm when we have discrete information as node features.

The result generalizes to graphs: if the WL algorithm does not distinguish (non-isomorphic) graphs G_1 and G_2, then any GNN (with the form as above) is incapable of distinguishing G_1 and G_2.

WL algorithm and GNNs (continue)

Theorem

There exists a GNN with the form defined in the previous theorem such that $\mathbf{h}_u^{(K)} = \mathbf{h}_v^{(K)}$ *only if* u *and* v *have the same labels after* K *iterations of the WL algorithm.*

Informally: there are GNNs that are *as powerful as* the WL algorithm.

Which GNNs are as powerful as the WL algorithm?

- the basic GNN? YES!
- basic GNN with neighborhood normalization? NO!
- GCN? NO!
- GraphSAGE? depends on the `AGGREGATION` operator

Graph Isomorphism Networks (GINs)

Xu, Keyulu, et al. "How powerful are graph neural networks?" *ICLR 2019*.
Update of a node:

$$\mathbf{h}_u^{(k+1)} = \texttt{MLP}^{(k)}\left(\left(1+\varepsilon^{(k)}\right)\mathbf{h}_u^{(k)} + \sum_{v\in\mathcal{N}(u)} \mathbf{h}_v^{(k)}\right)$$

where $\varepsilon^{(k)}$ is learnable parameter.

GIN has the maximal representational power for a (message-passing) GNN: if two graphs can be distinguished by GIN, they can be also distinguished by the WL algorithm, and vice versa

GNNs for Node Embeddings

In general: GNNs can be used to obtain node embeddings.

In terms of the encoder-decoder framework:

- *encoder*: GNN
- *similarity function*: see the ones for shallow embeddings
- *decoder*: see the ones for shallow embeddings
- *loss*: see the ones for shallow embeddings

task-dependent GNN

However: GNNs can also be used for *supervised* tasks.

GNNs for Supervised-Tasks

Common supervised tasks for graphs:

- node classification
- graph classification

GNNs: Node Classification

Input: some nodes have a label and can be used to train the GNN.

Each node u in the training set has a label, encode by a $0-1$ vector $\mathbf{y}_u$ of dimension c.

Loss function: negative log-likelihood loss of softmax classification function

Given the embedding $\mathbf{z}_u$ of node u and the corresponding vector $\mathbf{y}_u$, the softmax classification function is

$$\text{softmax}(\mathbf{z}_u, \mathbf{y}_u) = \sum_{i=1}^{c} \mathbf{y}_u[i] \frac{e^{\mathbf{z}_u^T \mathbf{w}_i}}{\sum_{j=1}^{c} e^{\mathbf{z}_u^T \mathbf{w}_j}}$$

linear model per label i

input: embedding z_u

unico termine, di label corretta

with $\mathbf{w}_i$ for $i = 1, \ldots, c$ trainable parameters.

GNNs: Node Classification (continue)

Then the loss function is:

$$\mathcal{L} = \sum_{u \in V_{\text{train}}} -\log\left(\text{softmax}(\mathbf{z}_u, \mathbf{y}_u)\right)$$

where V_{train} is the set of *training nodes*.

Note: there are different types of nodes for node classification

- the set V_{train} of *training nodes*: both the nodes and the labels are used during training (i.e., to learn the GNN parameters)
- the set V_{trans} of transductive test nodes: the nodes, but not their labels, are used during training. These nodes do not (directly) contribute to $\mathcal{L}$ ⇒ non considerarli potrebbe cambiare altri embedding
- the set V_{ind} of inductive test nodes: the nodes are completely *unobserved* during training

GNNs: Graph Classification

Input: set of graphs, where each graph G has a label represented by a $0-1$ vector $\mathbf{y}_G$ of dimension c

Loss: same as for node classification, where the embedding $\mathbf{z}_G$ is computed for a graph G.

$$\text{softmax}(\mathbf{z}_G, \mathbf{y}_G) = \sum_{i=1}^{c} \mathbf{y}_G[i] \frac{e^{\mathbf{z}_G^T \mathbf{w}_i}}{\sum_{j=1}^{c} e^{\mathbf{z}_G^T \mathbf{w}_j}}$$

$$\mathcal{L} = \sum_{G \in \mathcal{G}_{\text{train}}} -\log\left(\text{softmax}(\mathbf{z}_G, \mathbf{y}_G)\right)$$

where $\mathcal{G}_{\text{train}}$ is the set of graphs used for training.

GNNs: other tasks

GNNs can be used for several other tasks

- edge prediction: predict *missing edges*
- regression task for nodes
- regression task for graphs

GNNs: Additional Notes

What algorithm is used to learn GNN parameters? **SGD**

Training all nodes of a GNN simultaneously can require a lot of resources (time, memory) $\Rightarrow$ **Mini-batching:** obtain the final representation z_u for a small set of nodes at the time

Problem: how do we make sure that the computation graph is connected but not all nodes are used? $\Rightarrow$ Start from the target nodes and use **subsampling**: sample a fixed number of neighbours for each node.

The loss function can be combined with *regularization* (e.g., ℓ_2 regularization)

GNNs: Frameworks

If you are starting to use GNNs, here are some pointers to GNN Python libraries:

PyTorch Geometric
https://pytorch-geometric.readthedocs.io/en/latest/

Deep Graph Library https://www.dgl.ai/

Graph Nets https://github.com/deepmind/graph_nets

Spektral https://graphneural.network/