What is Geometric Deep Learning?

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Pytorch Geometric tutorials

- Antonio Longa and Gabriele Santin
- Open source project

- Learn how to use Geometric Deep Learning
- Pytorch Geometric

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How it works

- Brief introduction to a GDL model
- Practice!
- Feel free to join, ask and present

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How it works

- Brief introduction to a GDL model
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Who are you?

- Researchers
- Students
- Engineers
- ...

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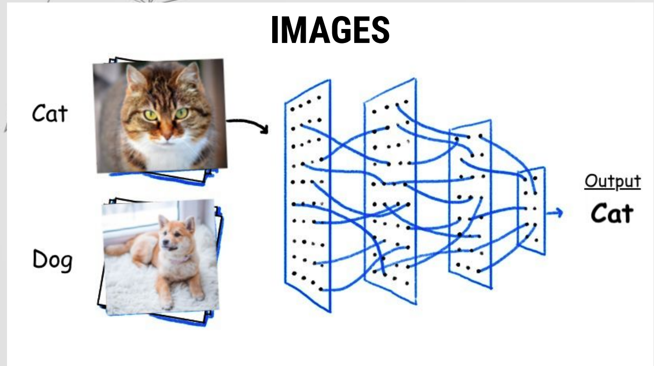
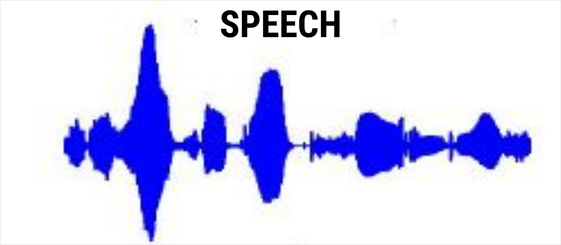
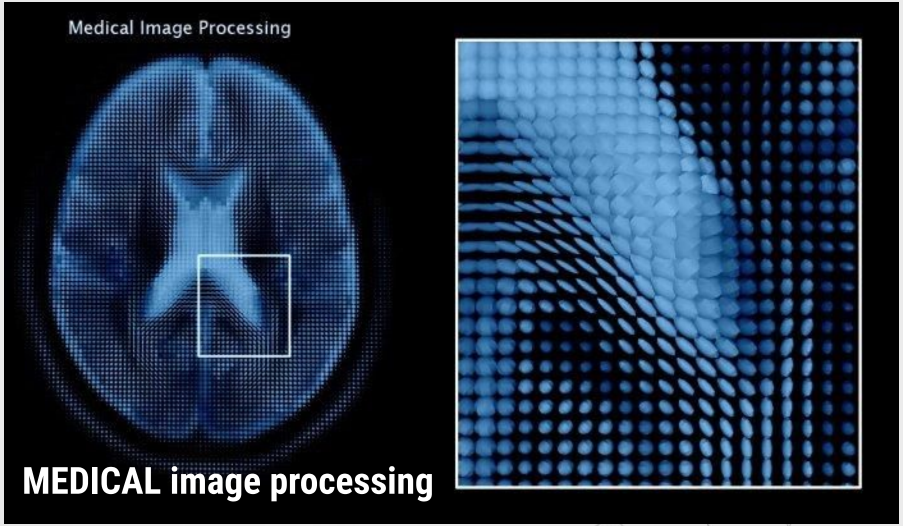
01 Deep Learning

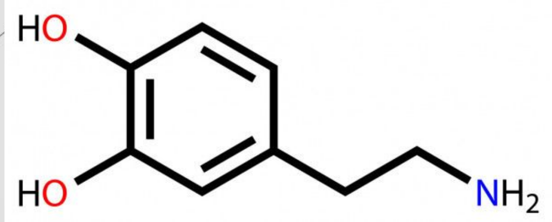




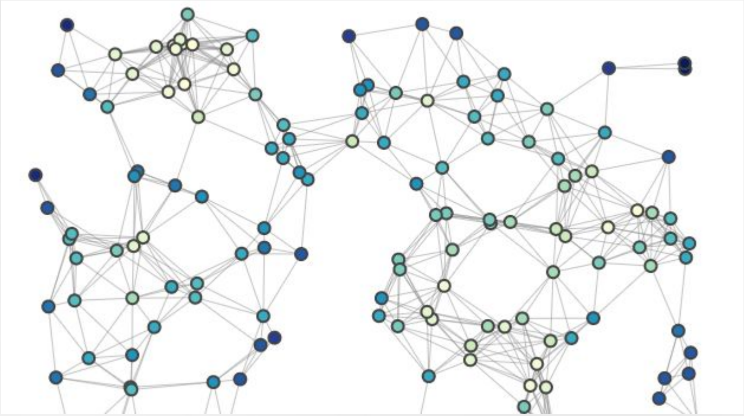


01 Other fields ?

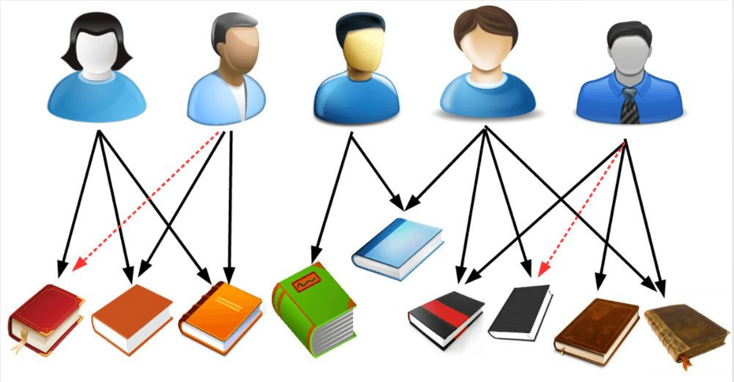
BIOLOGY



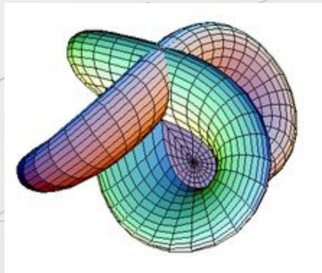
NETWORK Science



RECOMMENDER SYSTEMS



MANIFOLD



01 Other fields ?

DIFFERENCE BETWEEN:

- Images and manifold?
- Speech and molecules?
- RX images and graphs?

01 Other fields ?

DIFFERENCE BETWEEN:

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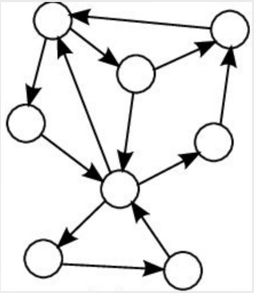
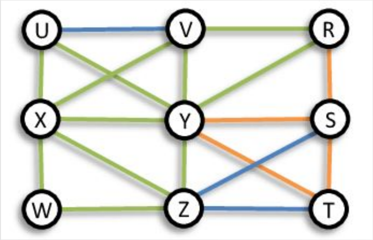
NON-EUCLIDEAN DOMAINS

02 Graphs

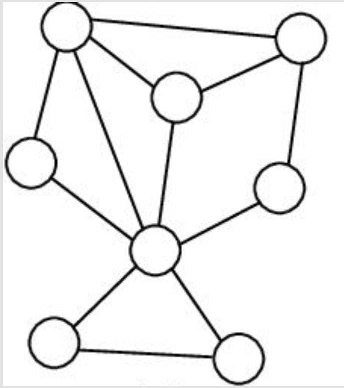
Directed



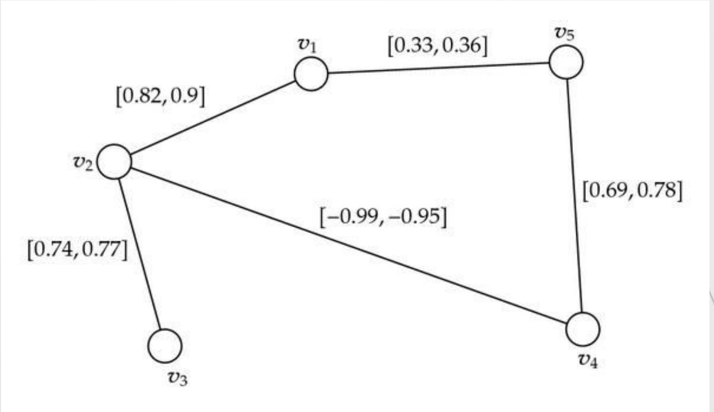
Node labeled graph



Undirected

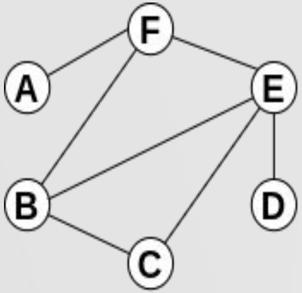


Edge labeled graph



03 Graph representation

GRAPH

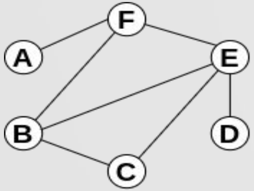


ADJ MATRIX

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

03 Deep learning

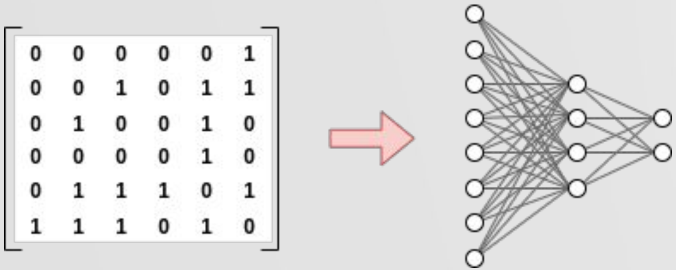
GRAPH



ADJ MATRIX

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

Neural network



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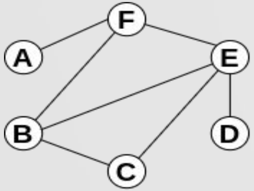
GRAPH



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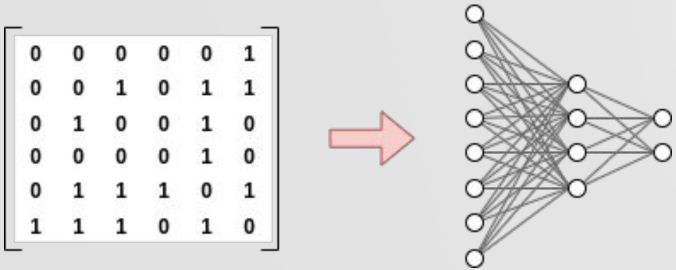
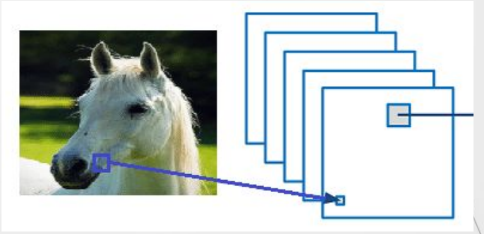
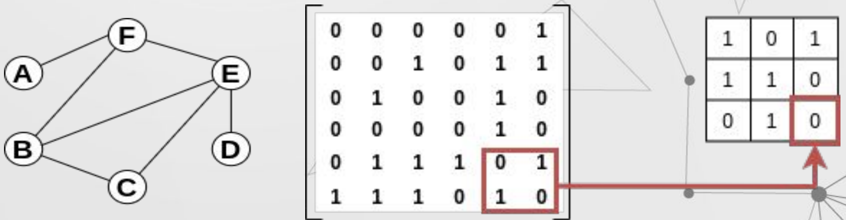
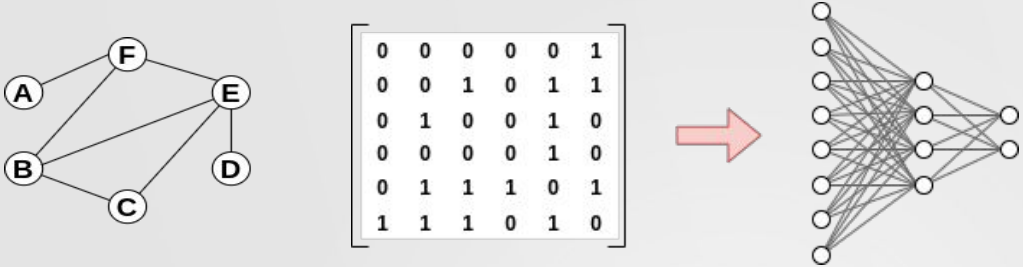


Convolution Neural network





03 Deep learning

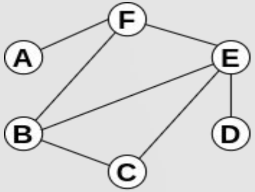


PROBLEMS:

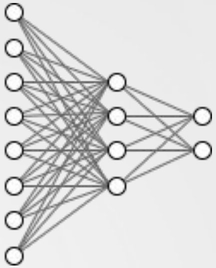
- Different sizes
- NOT invariant to nodes ordering

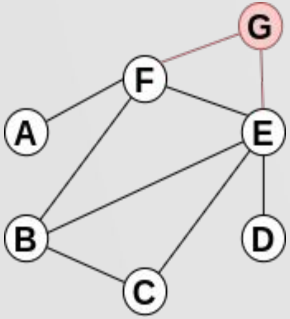
03 Deep learning: problems

Different sizes



$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$



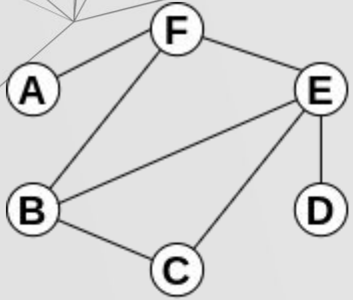


$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

03 Deep learning: problems

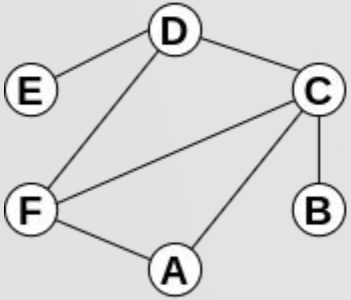
NOT invariant to node ordering

G



$$G = G'$$

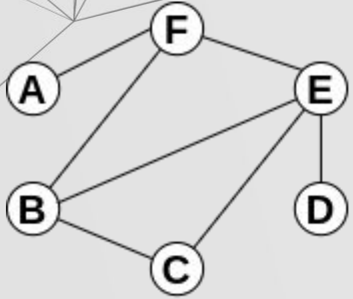
G'



03 Deep learning: problems

NOT invariant to node ordering

G

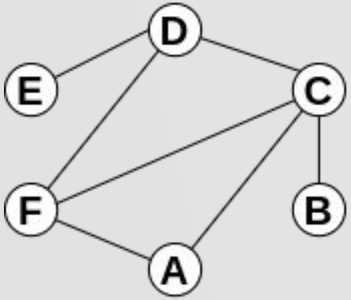


$$\mathrm{Adj}(G) \quad \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

$$G = G'$$

$$\mathrm{Adj}(G) \neq \mathrm{Adj}(G')$$

G'



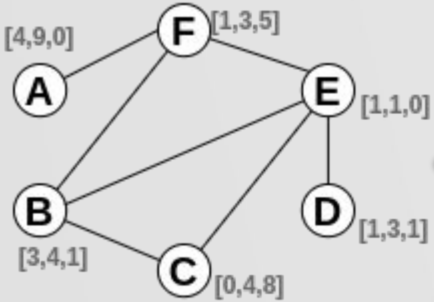
$$\mathrm{Adj}(G') \quad \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

04 Definitions

$$\mathbf{X} \in \mathcal{R}^{m \times |V|}$$

$$\begin{bmatrix} 4 & 9 & 0 \\ 3 & 4 & 1 \\ 0 & 4 & 8 \\ 1 & 3 & 1 \\ 1 & 1 & 0 \\ 1 & 3 & 5 \end{bmatrix}$$

$$\boldsymbol{G} = (V,E)$$



$$\mathbf{A} = \mathrm{Adj}(\boldsymbol{G})$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

05 Graph neural networks

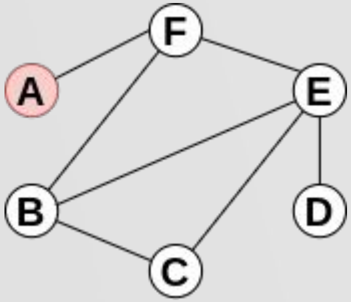
- Define a **computation graph**
- **Use** the computation graph

05 Graph neural networks

COMPUTATION GRAPH

The neighbour of a node define its computation graph

INPUT GRAPH



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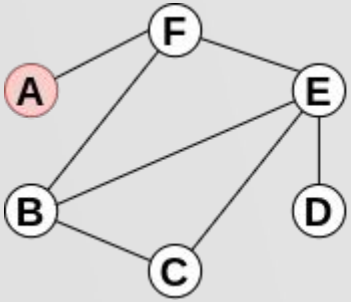

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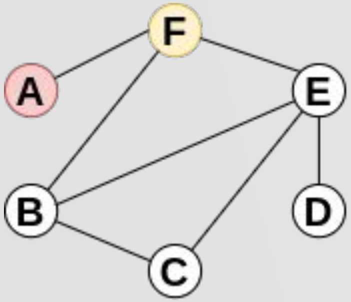

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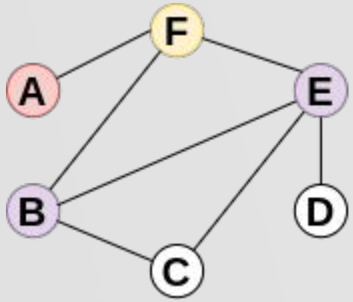

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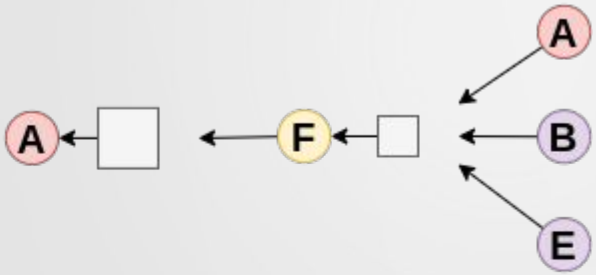

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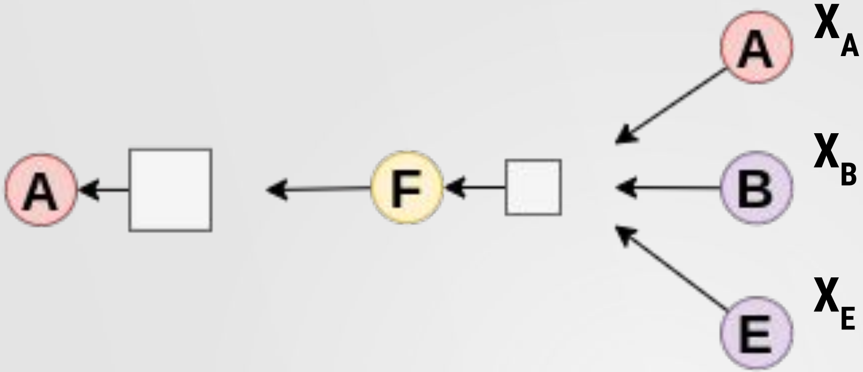

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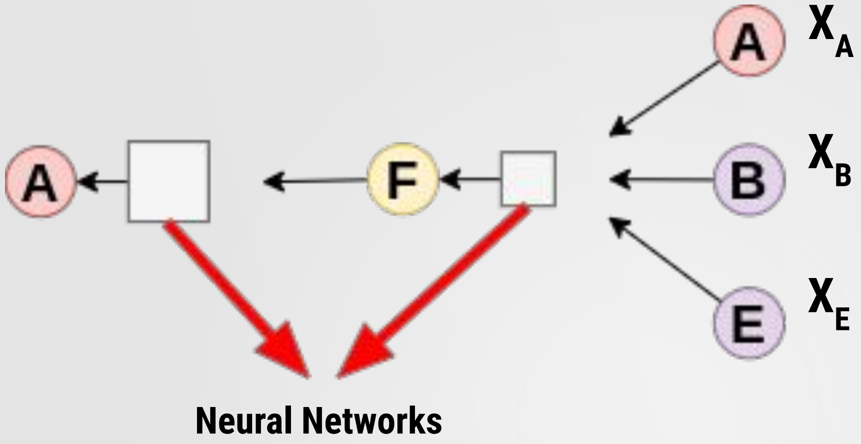

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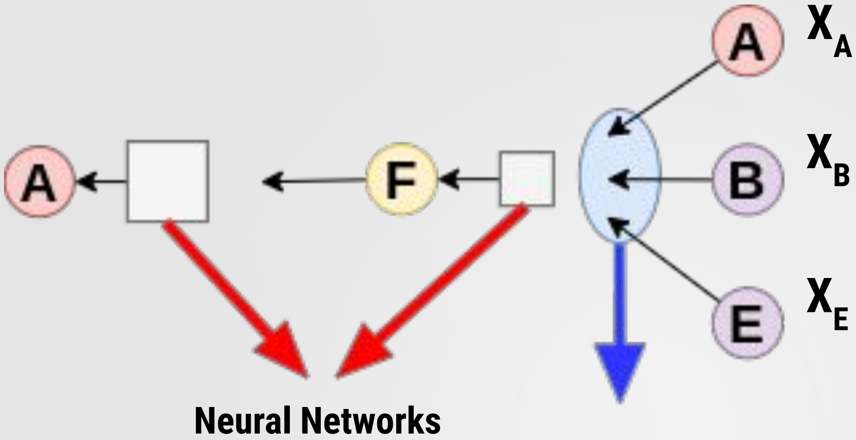
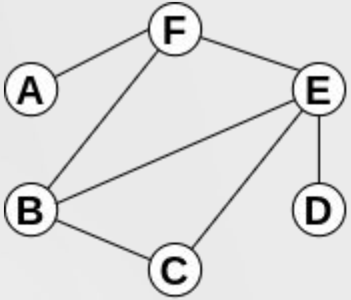


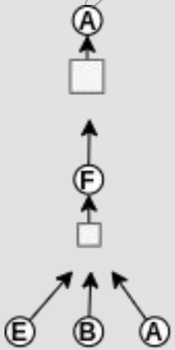
Ordering invariant
Aggregation

Sum
Average

05 Graph neural networks

Every node has its own **computation graph**





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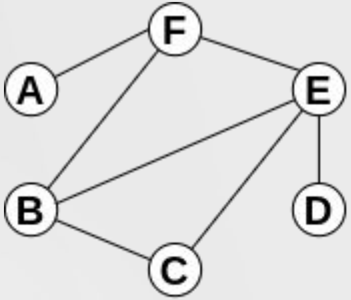

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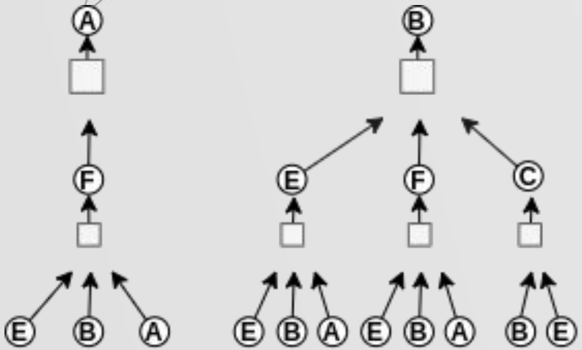

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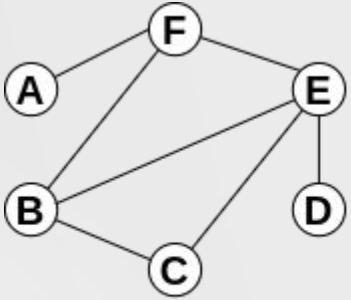

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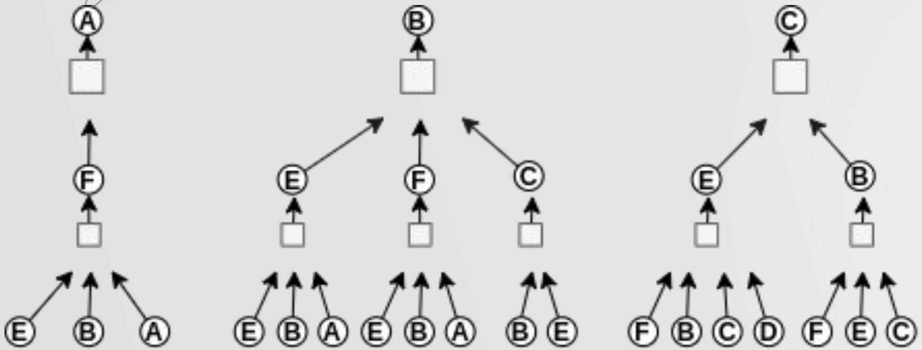

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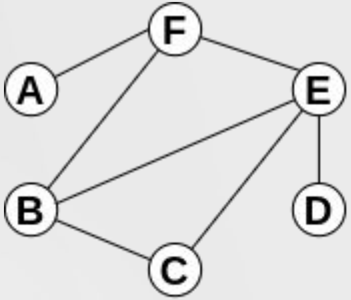

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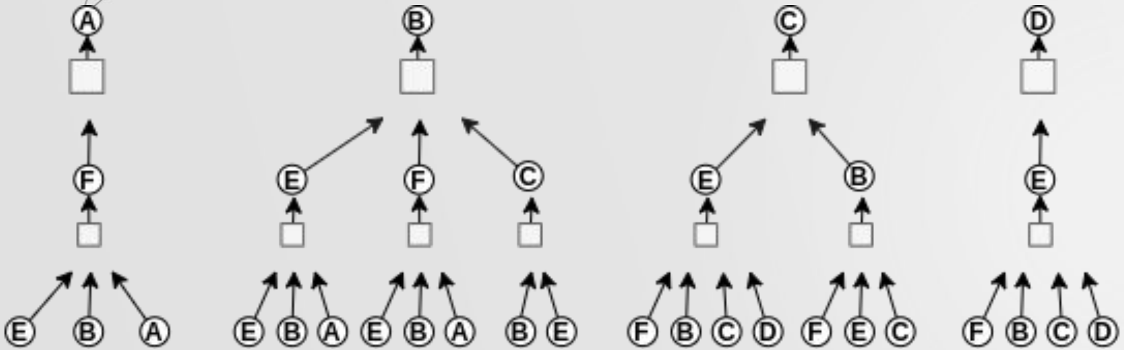

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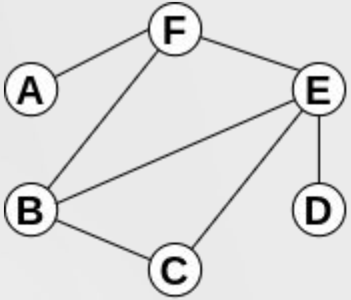

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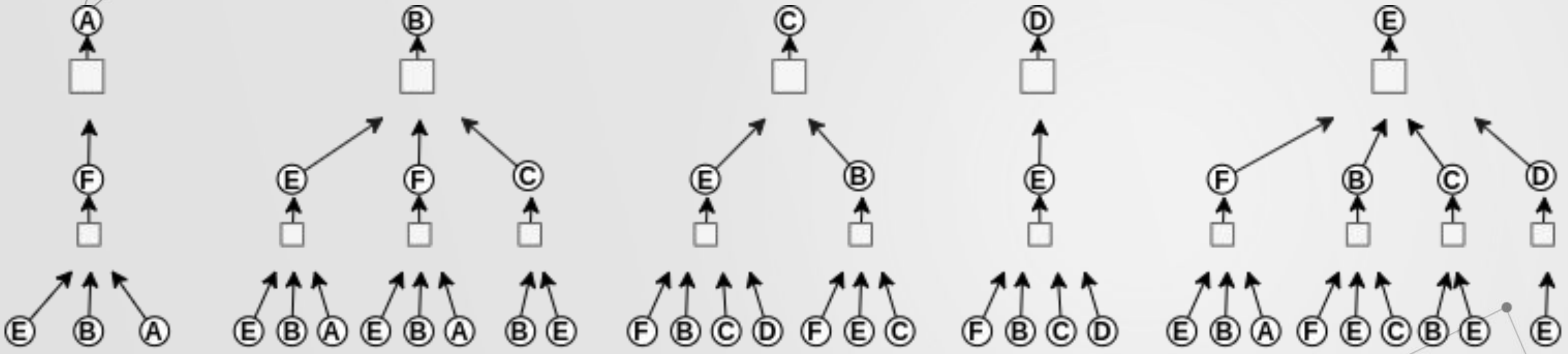

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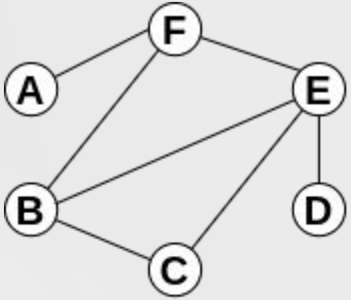

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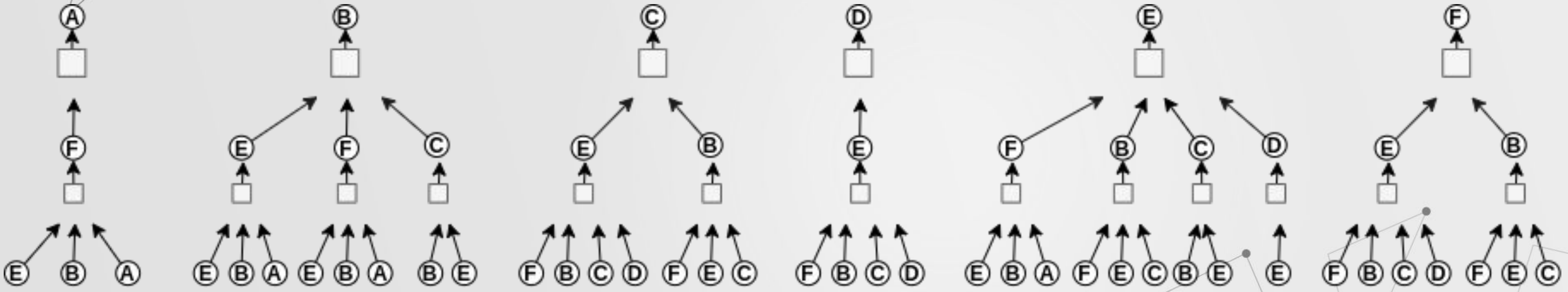
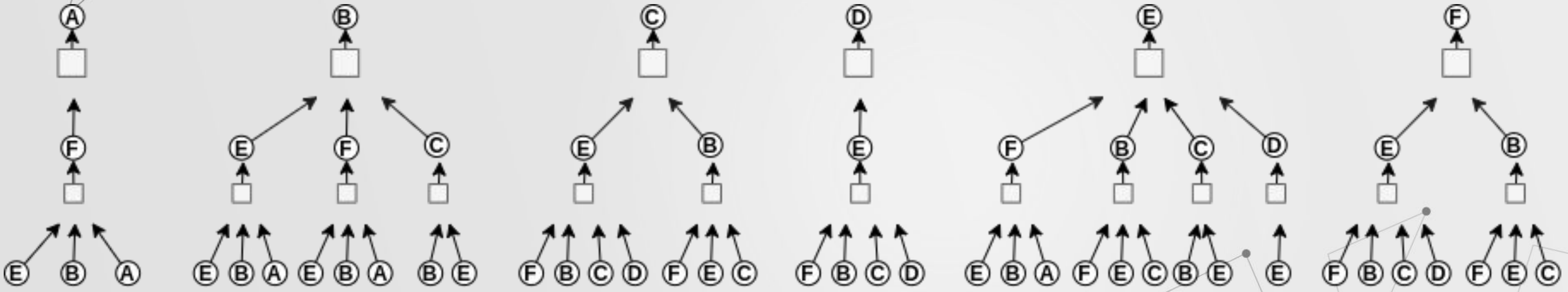


05 Graph neural networks

Can you see **redundancy?**



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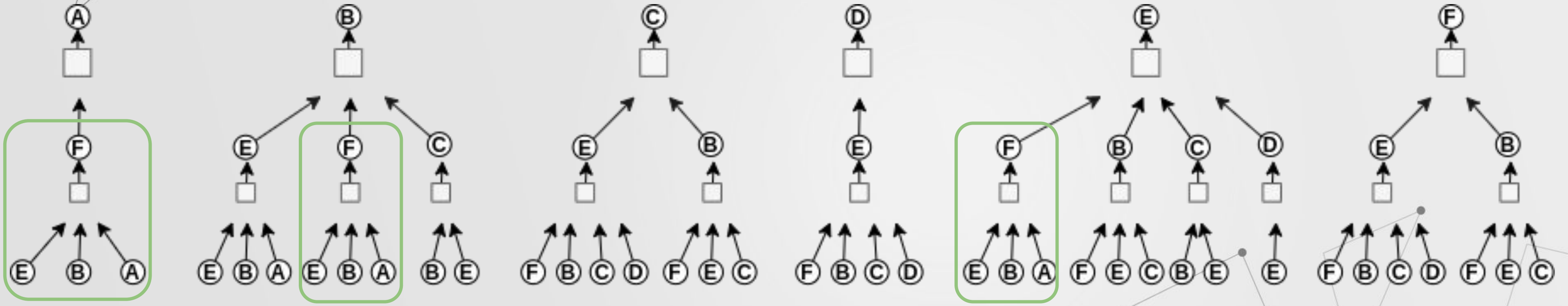

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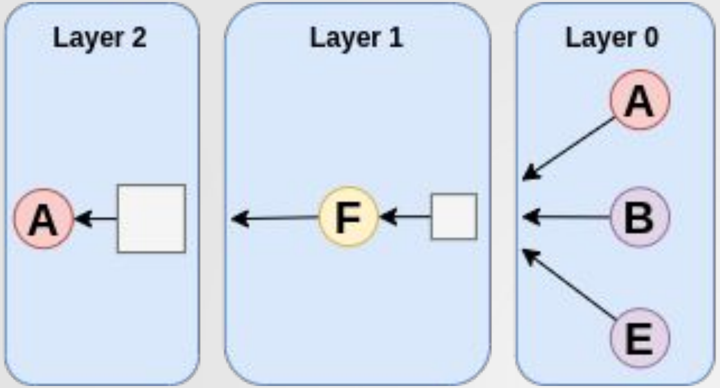
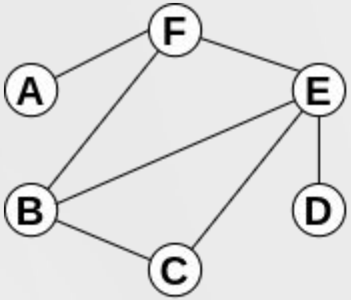
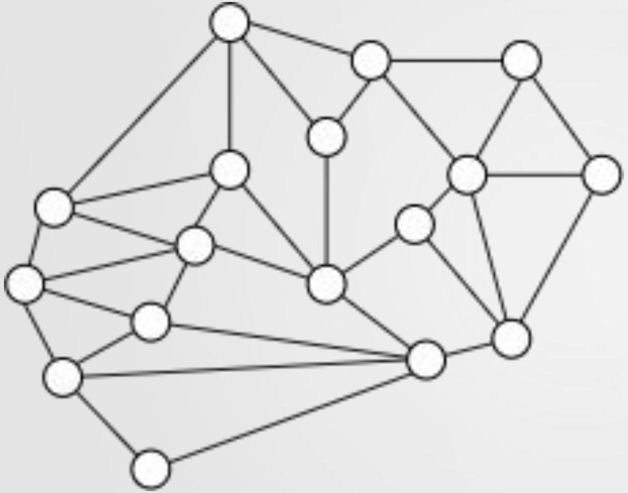




05 Graph neural networks

How much you have to **unroll**?



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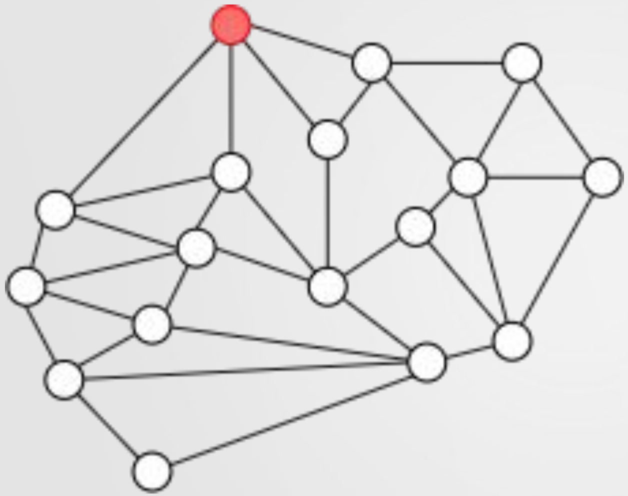

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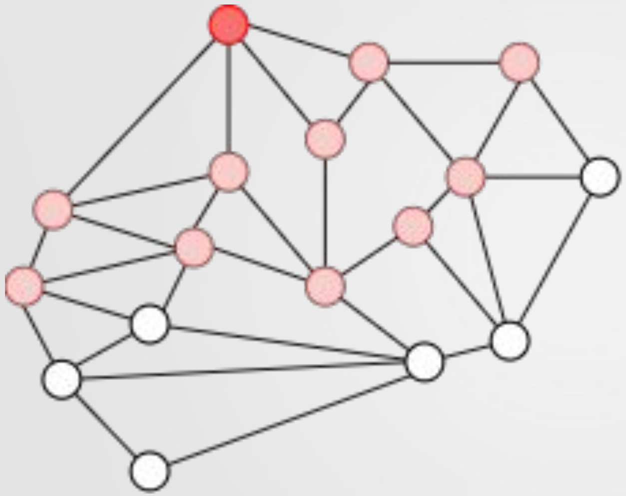
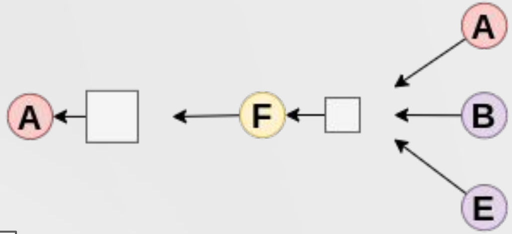


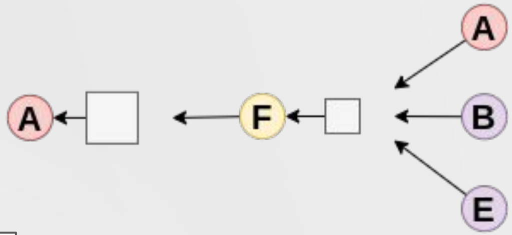
05 Graph neural networks

Math



$$H_v^0 = X_v$$

05 Graph neural networks

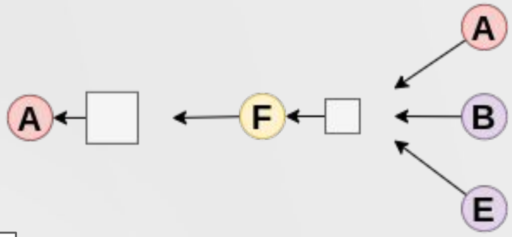


Math

$$H_v^0 = X_v$$

$$h_v^{k+1} = \sigma\left(W_k \sum_{u \in N(u)} \frac{h_u^k}{|N(v)|} + B_k h_v^k\right)$$

05 Graph neural networks



Math

$$H_v^0 = X_v$$

$$h_v^{k+1} = \sigma(W_k \sum_{u \in N(u)} \frac{h_u^k}{|N(v)|} + B_k h_v^k)$$

$$Z_v = h_v^K$$

05 Graph neural networks

$$h_v^{k+1} = \sigma(W_k \sum_{u \in N(u)} \frac{h_u^k}{|N(v)|} + B_k h_v^k)$$

05 Graph neural networks

$$h_v^{k+1} = \sigma(W_k \sum_{u \in N(u)} \frac{h_u^k}{|N(v)|} + B_k h_v^k)$$

It is the k+1 embedding of the node V

05 Graph neural networks

Embedding of node v, at the k-th embedding

$$h_v^{k+1} = \sigma\left(W_k \sum_{u \in N(u)} \frac{h_u^k}{|N(v)|} + B_k \boxed{h_v^k}\right)$$

It is the k+1 embedding of the node V

05 Graph neural networks

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It is the k+1 embedding of the node V

For each neighbour of v (**u = N(v)**), we average the embedding of the embedding at the k-th layer

05 Graph neural networks

Weights

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05 Graph neural networks

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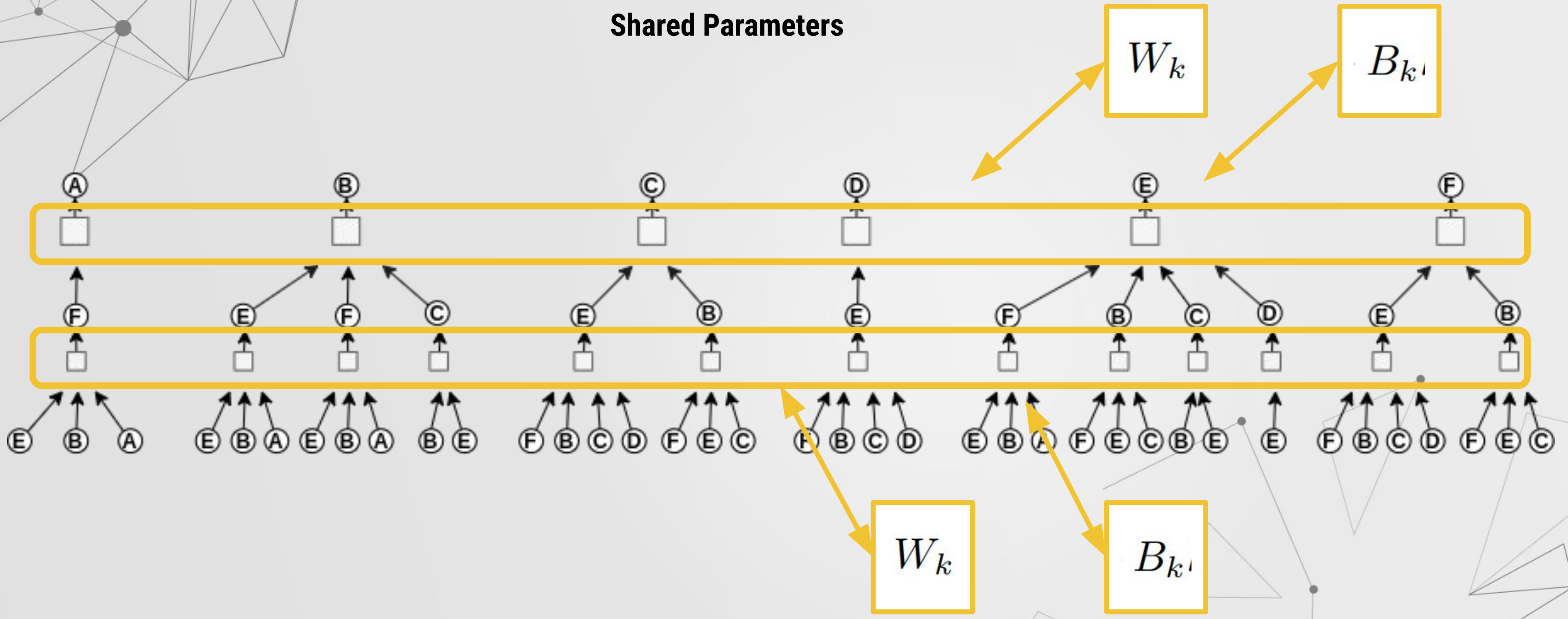
Activation function (**ReLU**)

For each neighbour of v (**u = N(v)**), we average the embedding of the embedding at the k-th layer

05 Graph neural networks

Shared Parameters



06 Graph SAGE

$$H_v^0 = X_v$$

$$h_v^{k+1} = \sigma(W_k \sum_{u \in N(u)} \frac{h_u^k}{|N(v)|} + B_k h_v^k)$$

$$Z_v = h_v^K$$

Inductive Representation Learning on Large Graphs

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06 Graph SAGE

$$h_v^{k+1} = \sigma(W_k \sum_{u \in N(u)} \frac{h_u^k}{|N(v)|} + B_k h_v^k)$$

$$h_v^{k+1} = \sigma([W_k \cdot AGG(\{h_u^{k-1}, \forall u \in N(v)\}), B_k h_v^k])$$

06 Graph SAGE

$$h_v^{k+1} = \sigma(W_k \boxed{\sum_{u \in N(u)} \frac{h_u^k}{|N(v)|}} + B_k h_v^k)$$

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06 Graph SAGE

$$h_v^{k+1} = \sigma([W_k \cdot \boxed{AGG}(\{h_u^{k-1}, \forall u \in N(v)\}), B_k h_v^k])$$

AGG:

- **AGG → POOL**: es: element-wise min/max
- **AGG → LSTM**: (note not order invariant)

07 Practice

Jupyter-notebook