Inductive Representation Learning on Large Graphs

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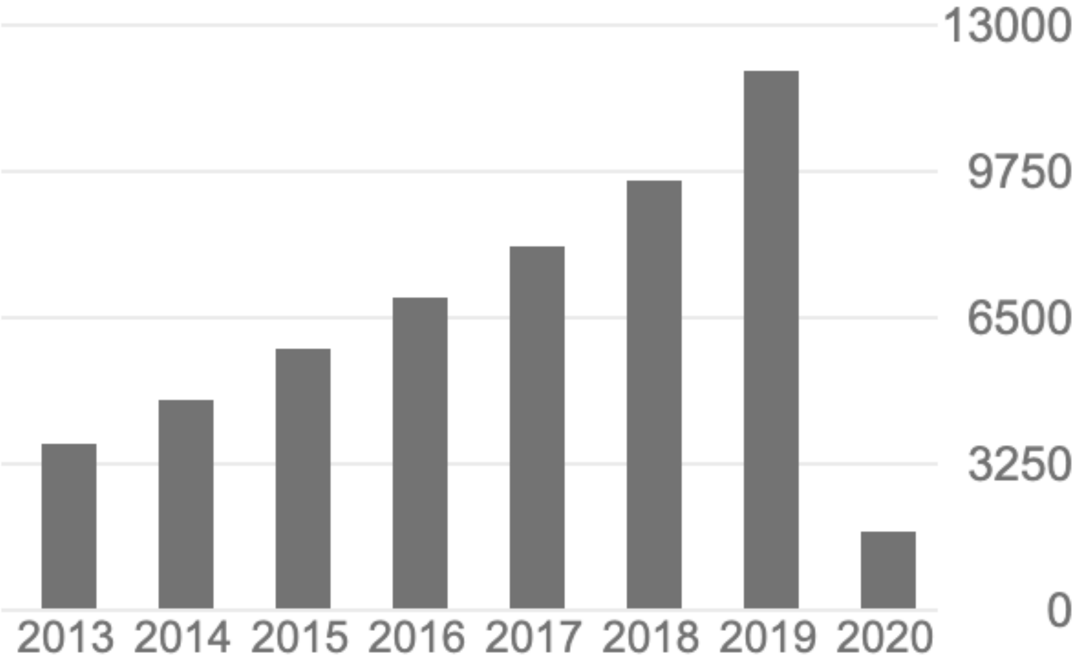

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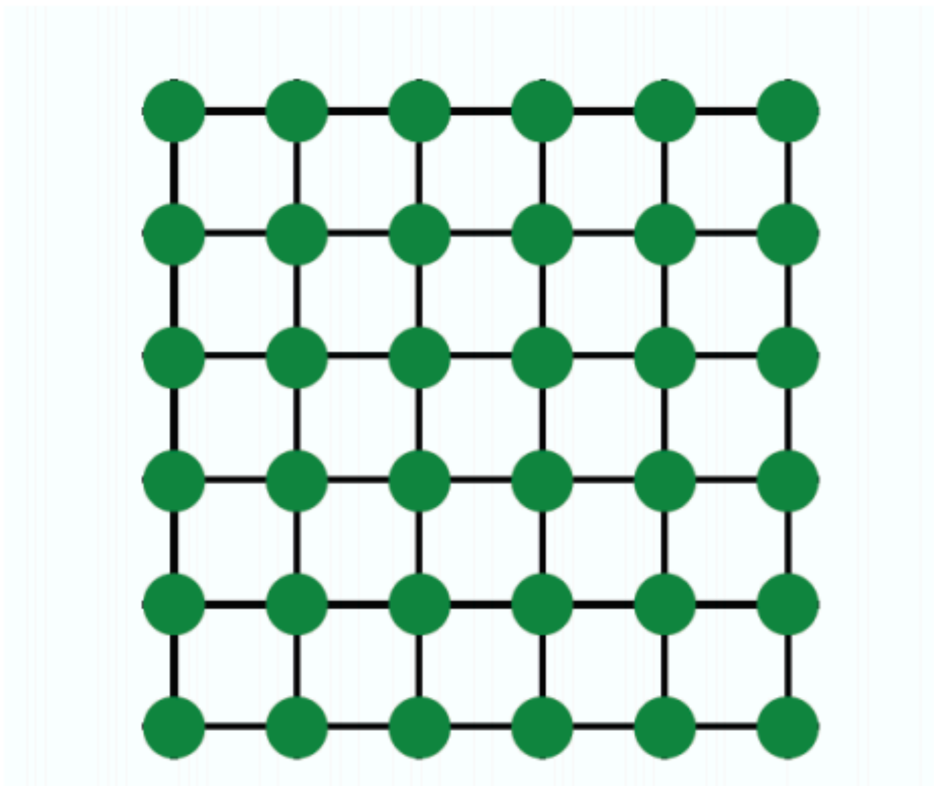
Modern Deep Learning



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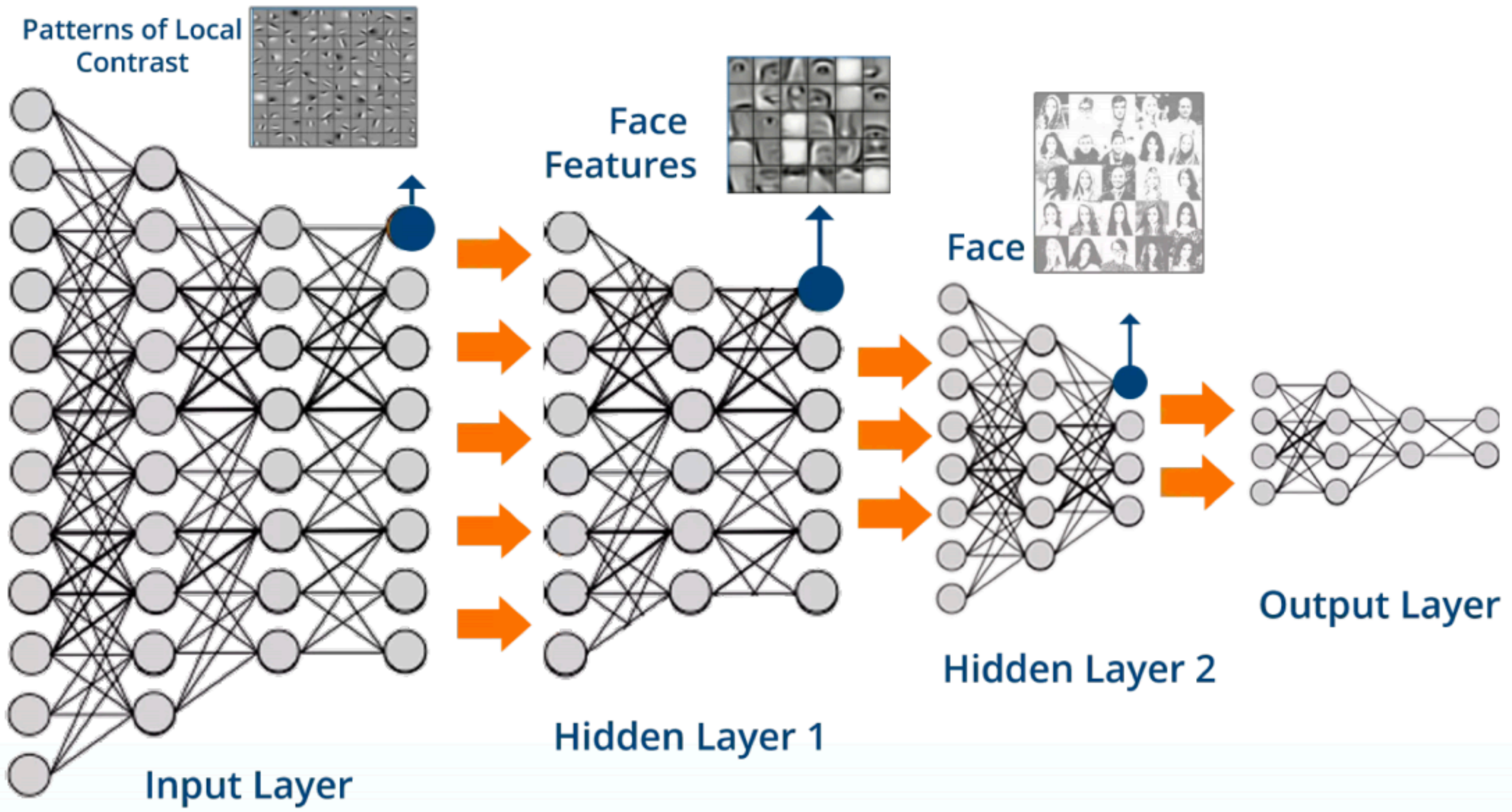

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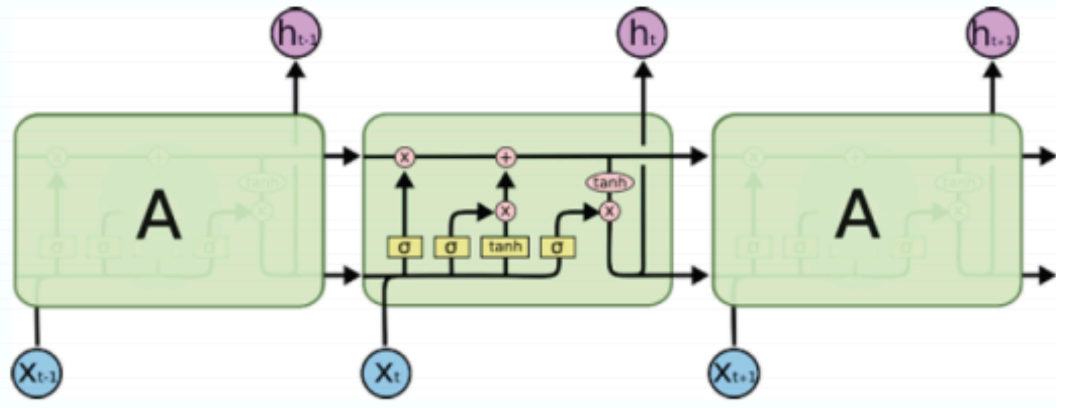
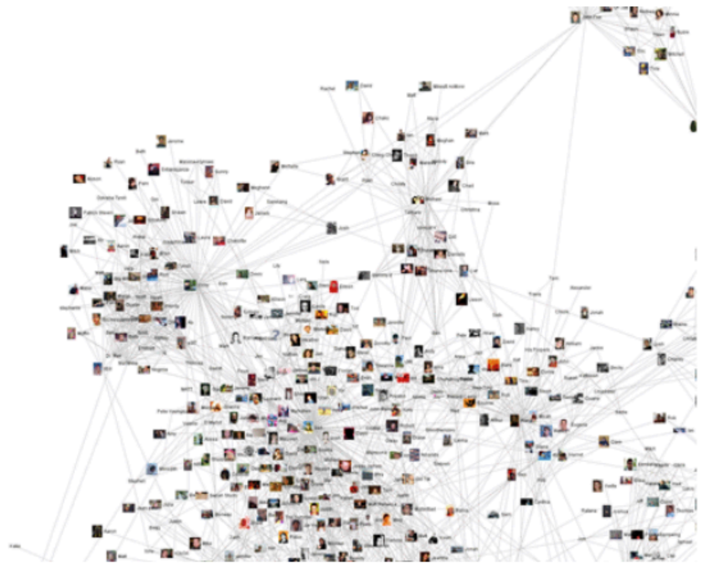


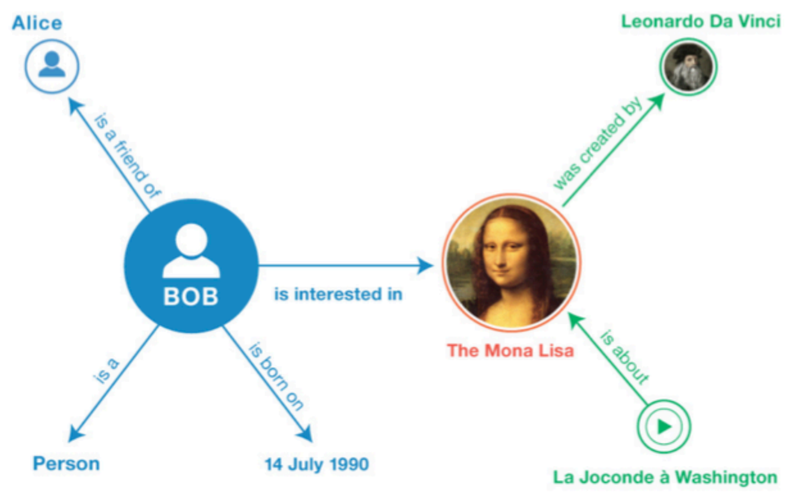
Modern deep learning toolbox is designed for simple sequences & grids

Networks

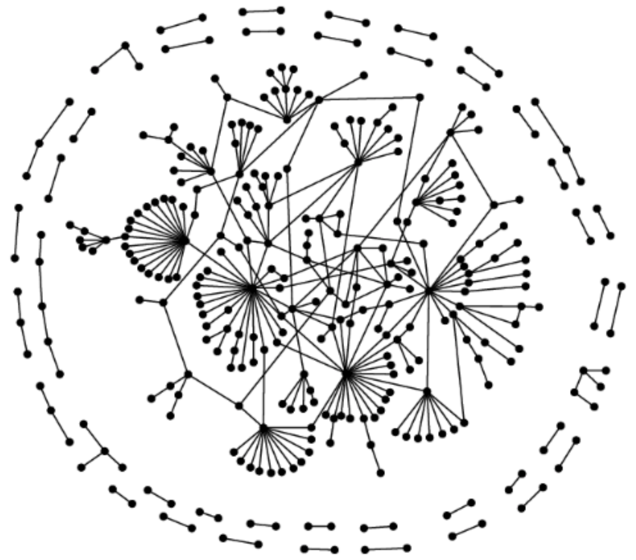
Not everything can be represented as a sequence or a grid



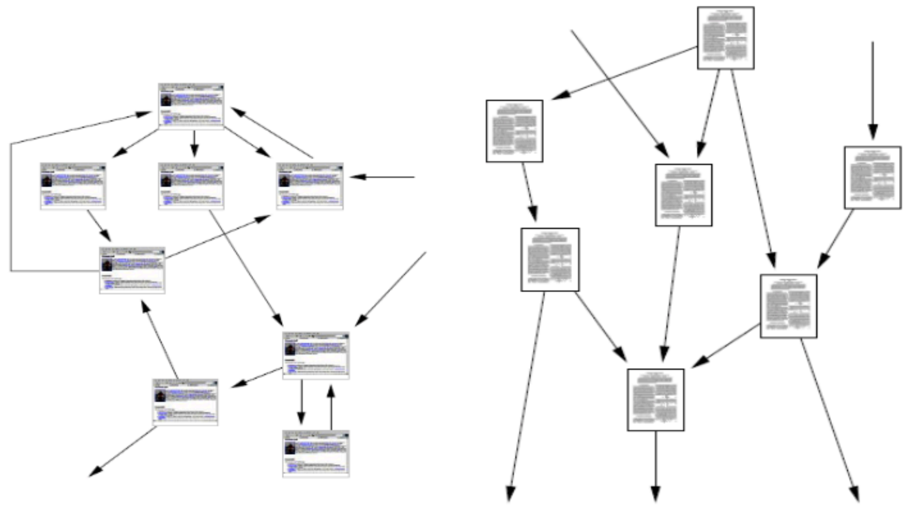
Social networks



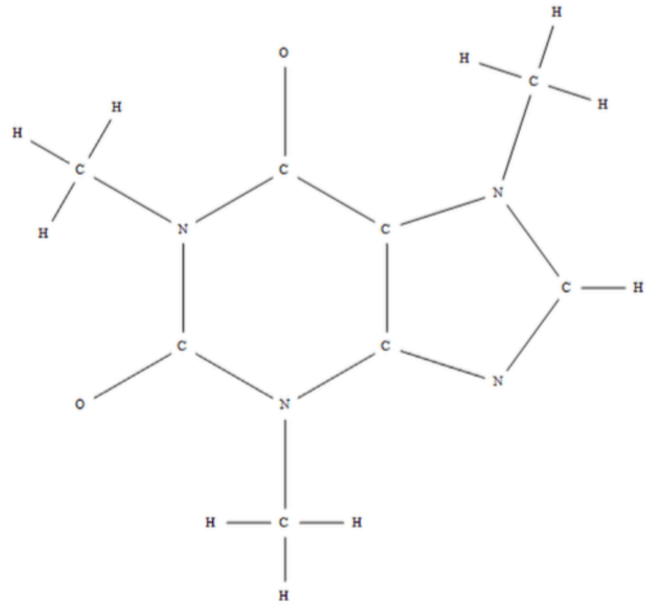
Knowledge graphs



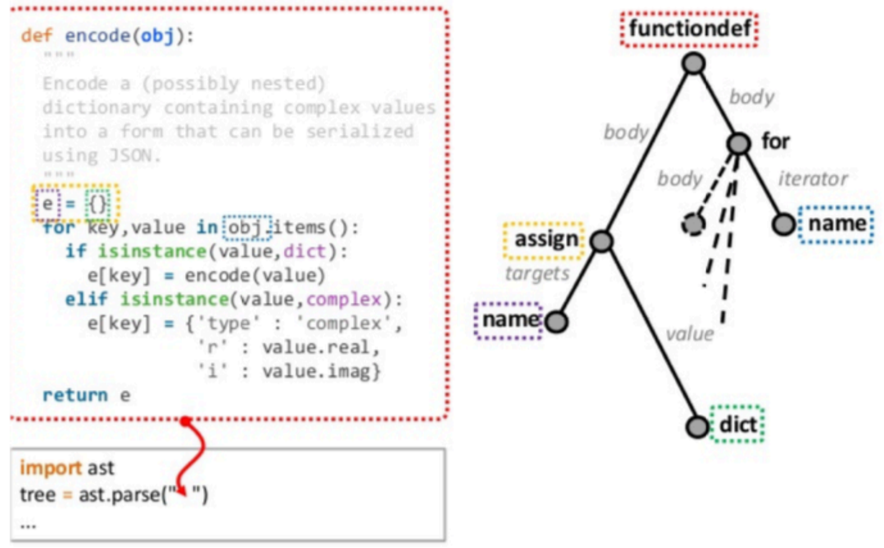
Biological networks



Complex Systems



Molecules

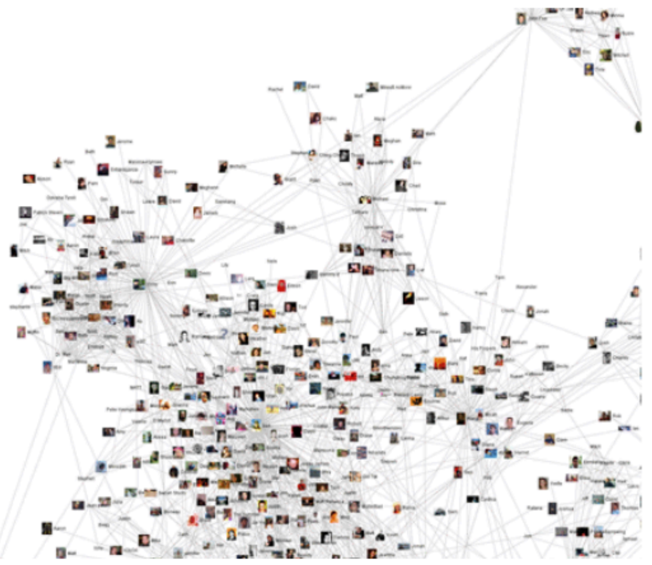


Code

Task

- Link prediction
- Node classification
- Community detection

Networks : Graph



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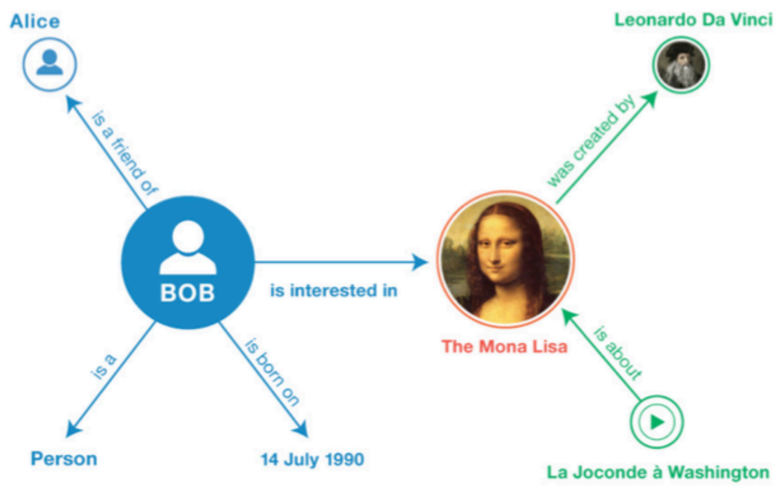
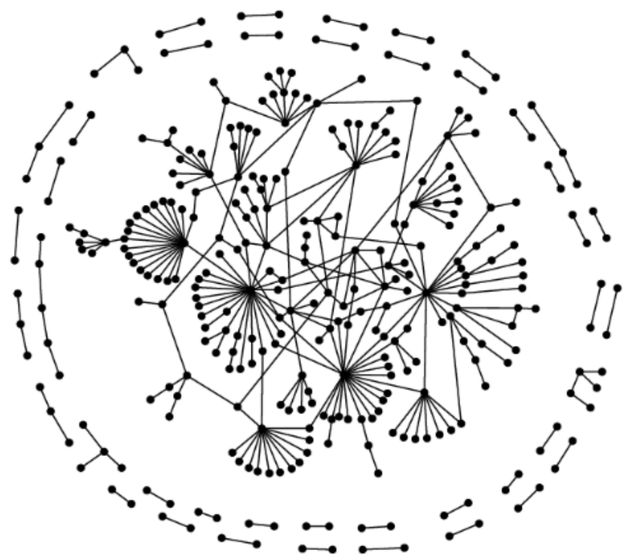


Knowledge graphs



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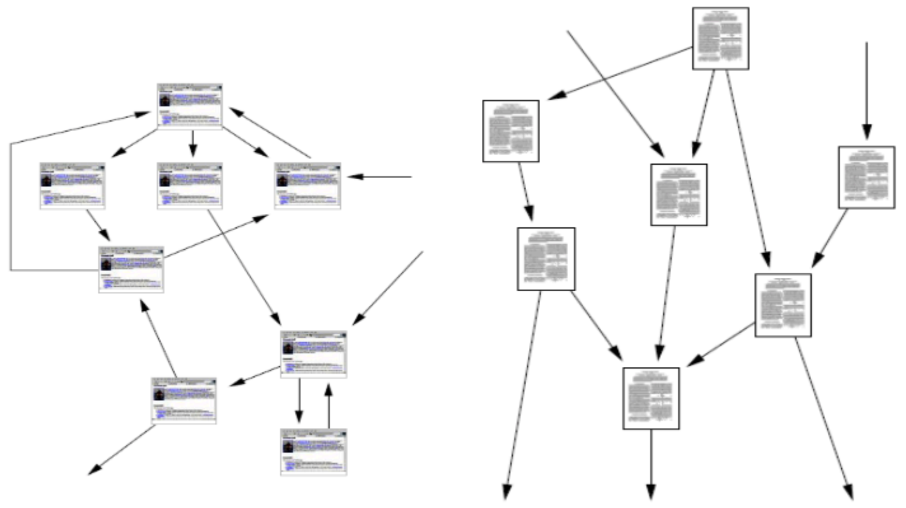
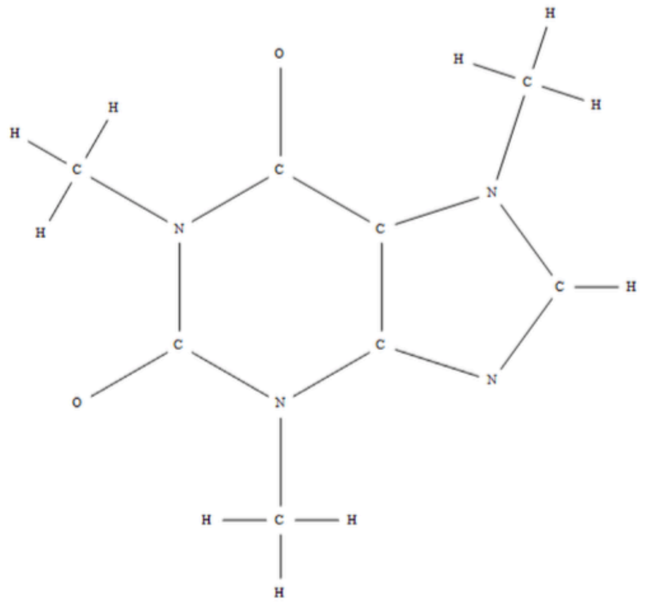
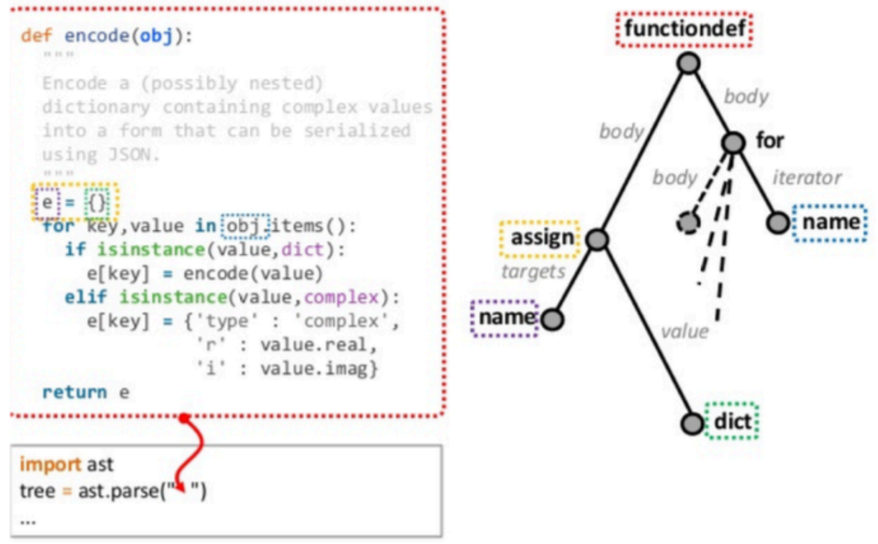


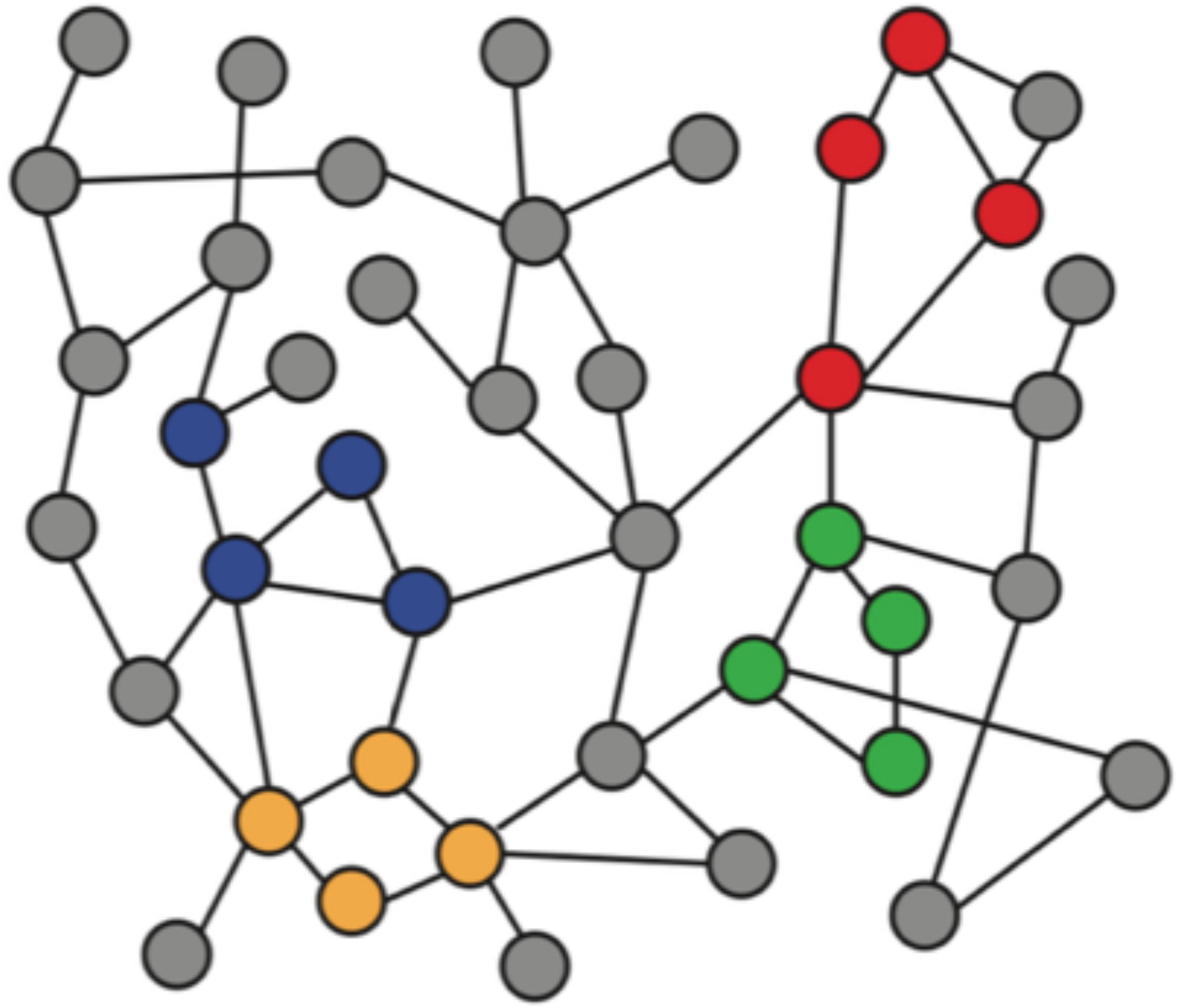
Complex Systems



Molecules



Code

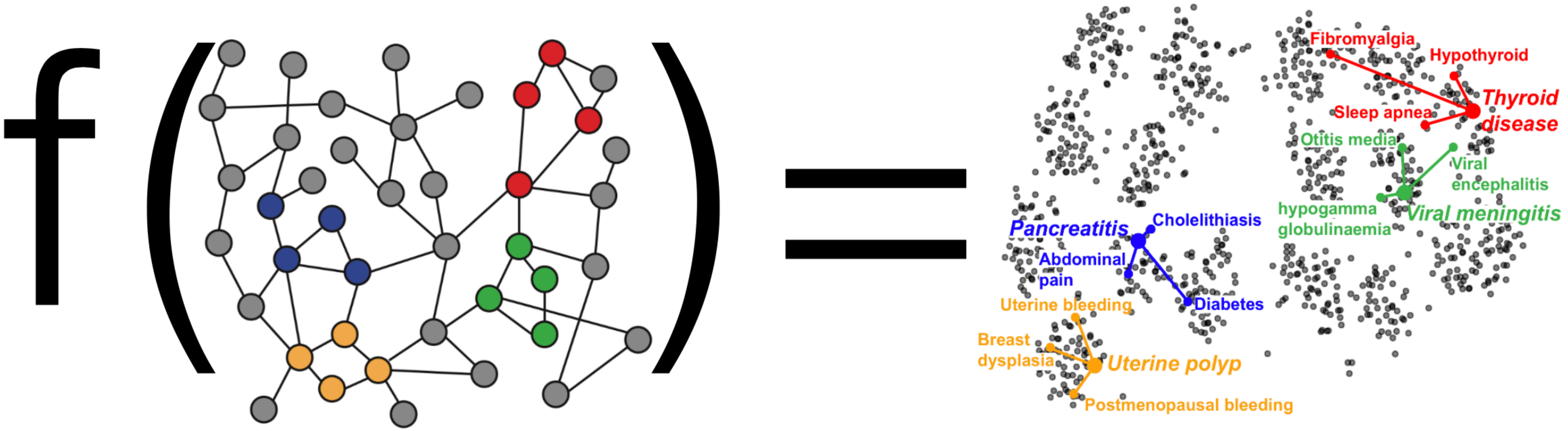


Abstract

Networks → Graph

Graph(node) Embedding

Map nodes to *d*-dimensional embeddings

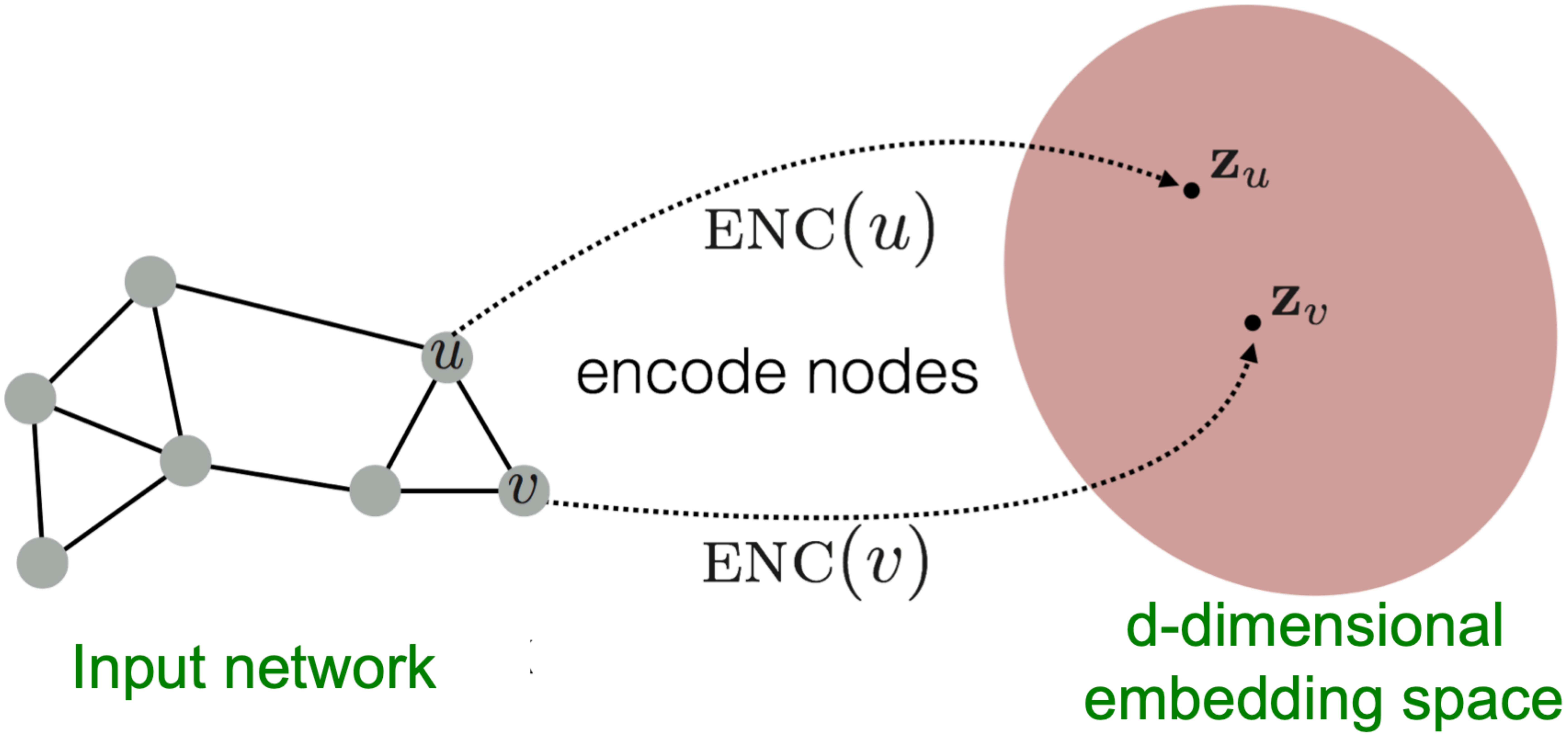


Input graph

2D node embeddings

How to learn mapping function f

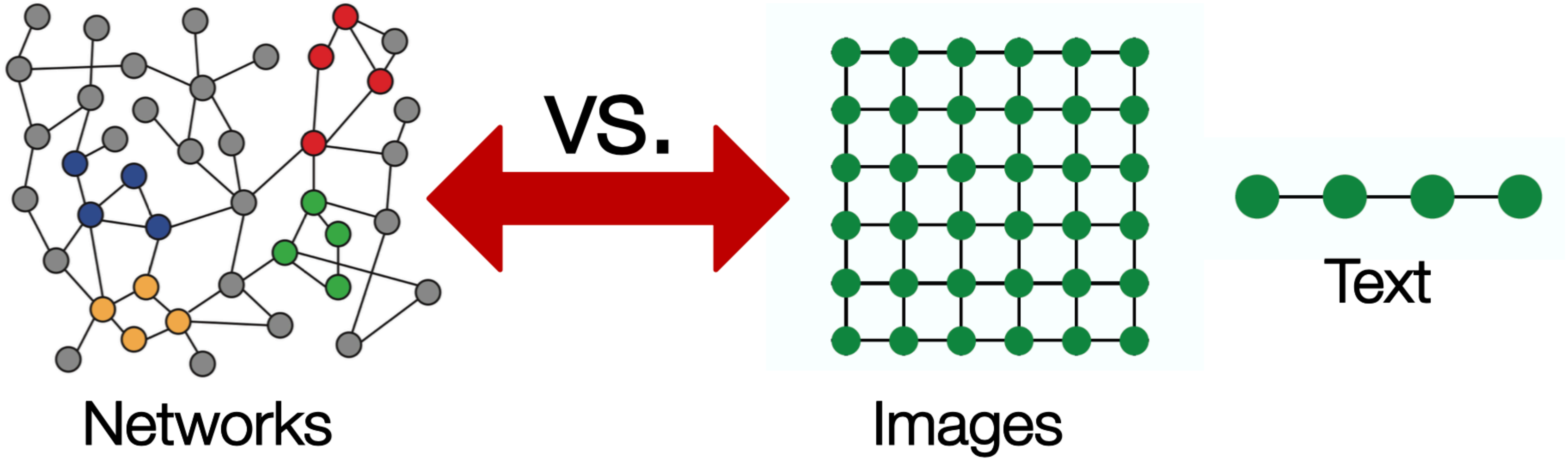
Embedding Rule



$$\textbf{similarity}\ (u, v) \approx \mathbf{z}_v^\top \mathbf{z}_u$$

In the network

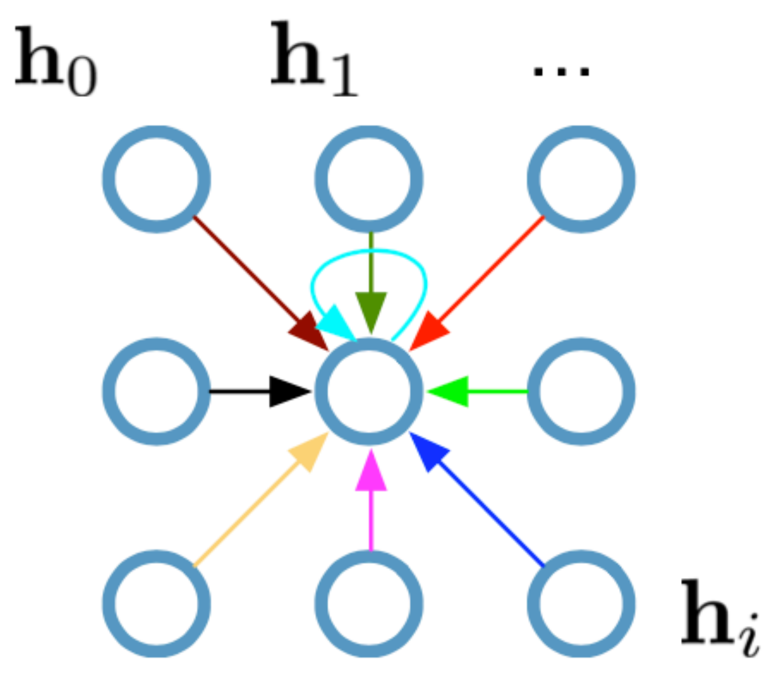
Hard : Networks are complex !



- 1. Arbitrary size and complex topological structure (no spatial locality)
- 2. No fixed node ordering or reference point
- 3. Often dynamic and have multimodal features

Idea : Convolutional Networks

Generalize convolutions from lattices to graph

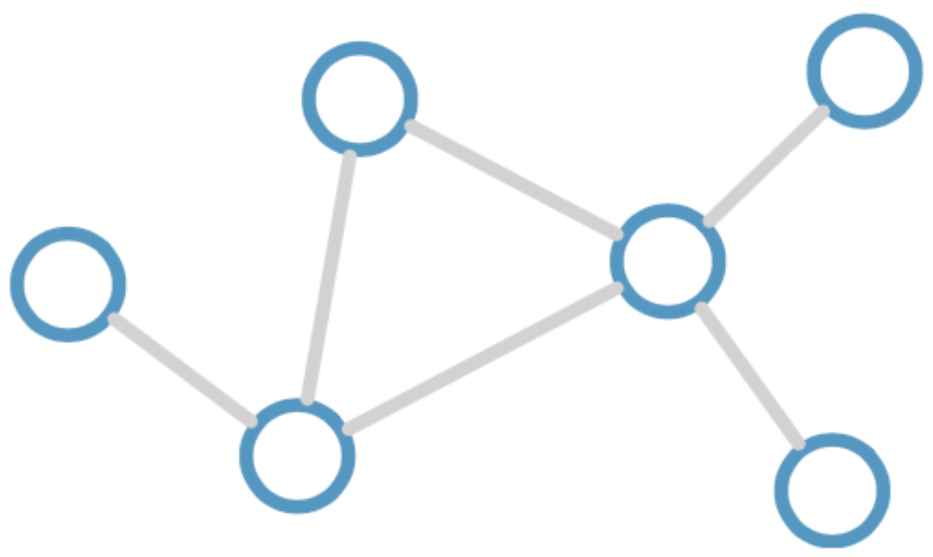


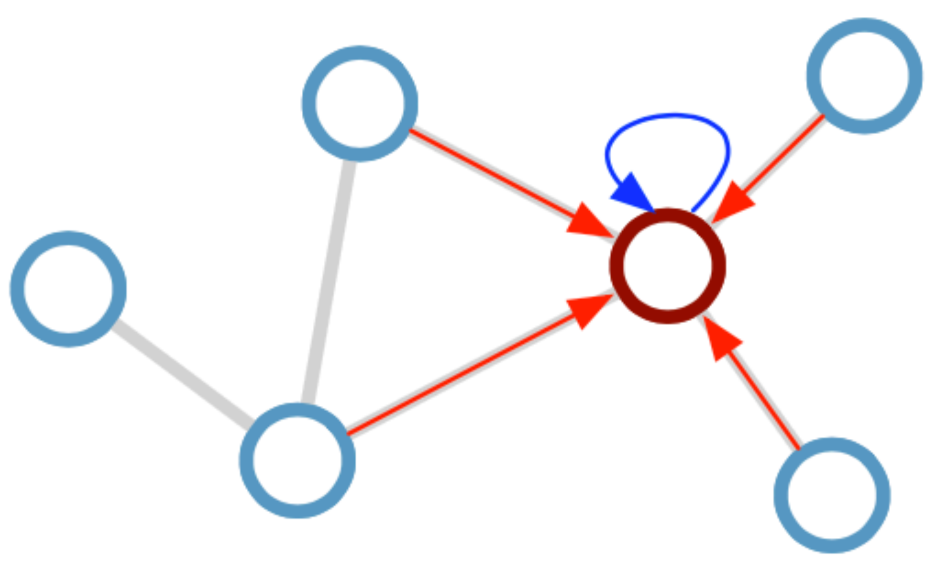
Update for a single pixel:

- Transform messages individually $\mathbf{W}_i \mathbf{h}_i$
- Add everything up $\sum_i \mathbf{W}_i \mathbf{h}_i$

Full update:

$$\mathbf{h}_4^{(l+1)} = \sigma\left(\mathbf{W}_0^{(l)}\mathbf{h}_0^{(l)} + \mathbf{W}_1^{(l)}\mathbf{h}_1^{(l)} + \cdots + \mathbf{W}_8^{(l)}\mathbf{h}_8^{(l)}\right)$$



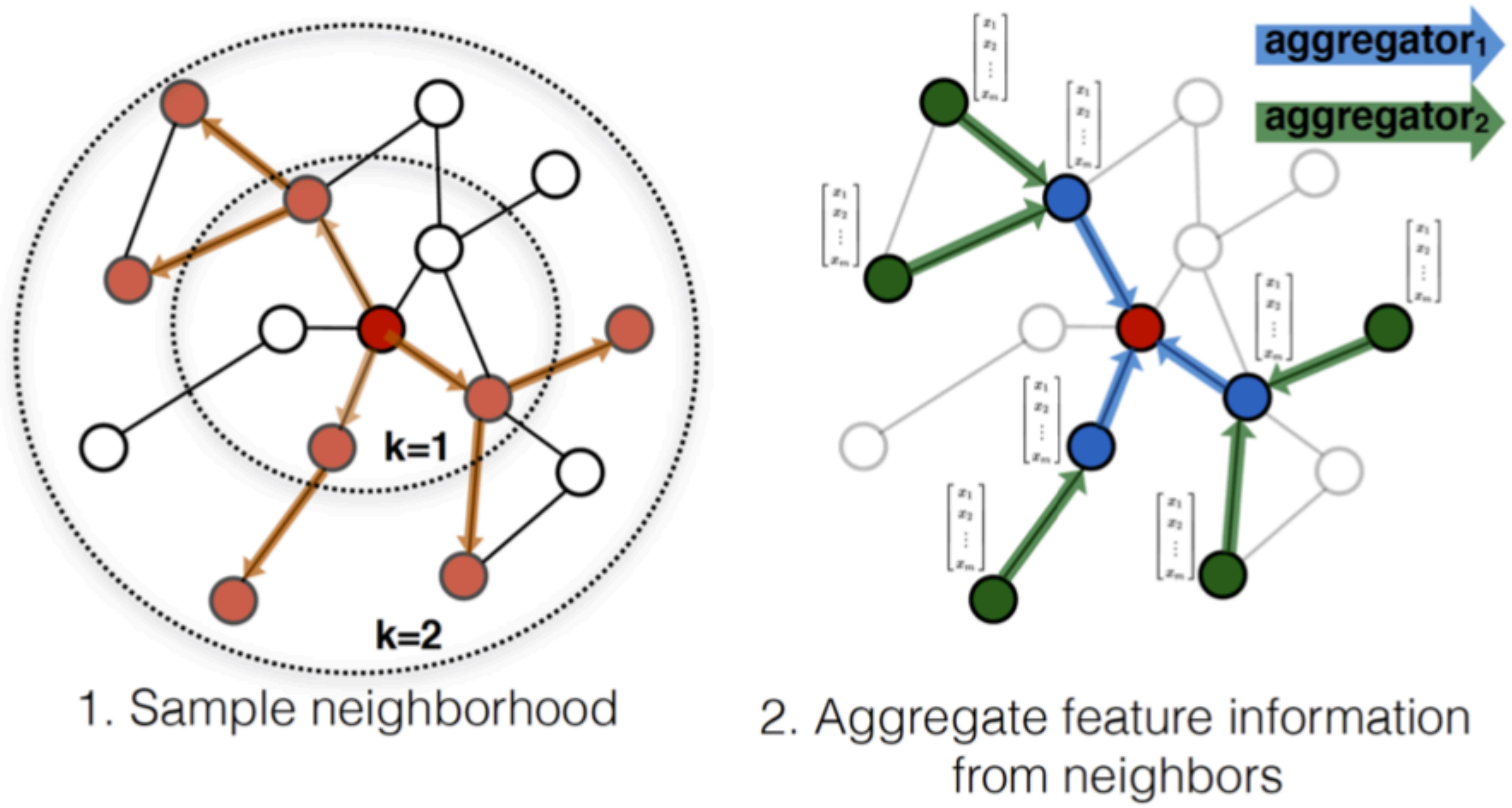


Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j \in \mathcal{N}_i} \frac{1}{c_{ij}} \mathbf{h}_j^{(l)} \mathbf{W}_1^{(l)}\right)$$

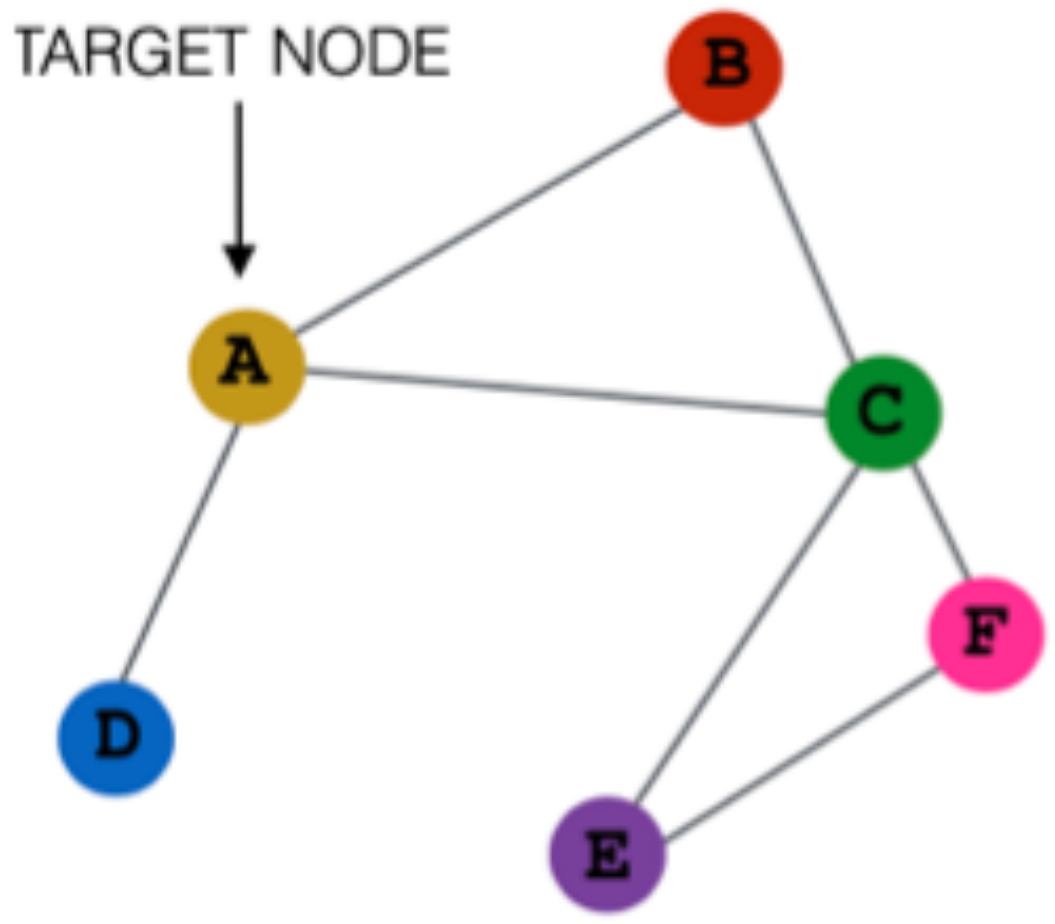
Approach : GraphSAGE

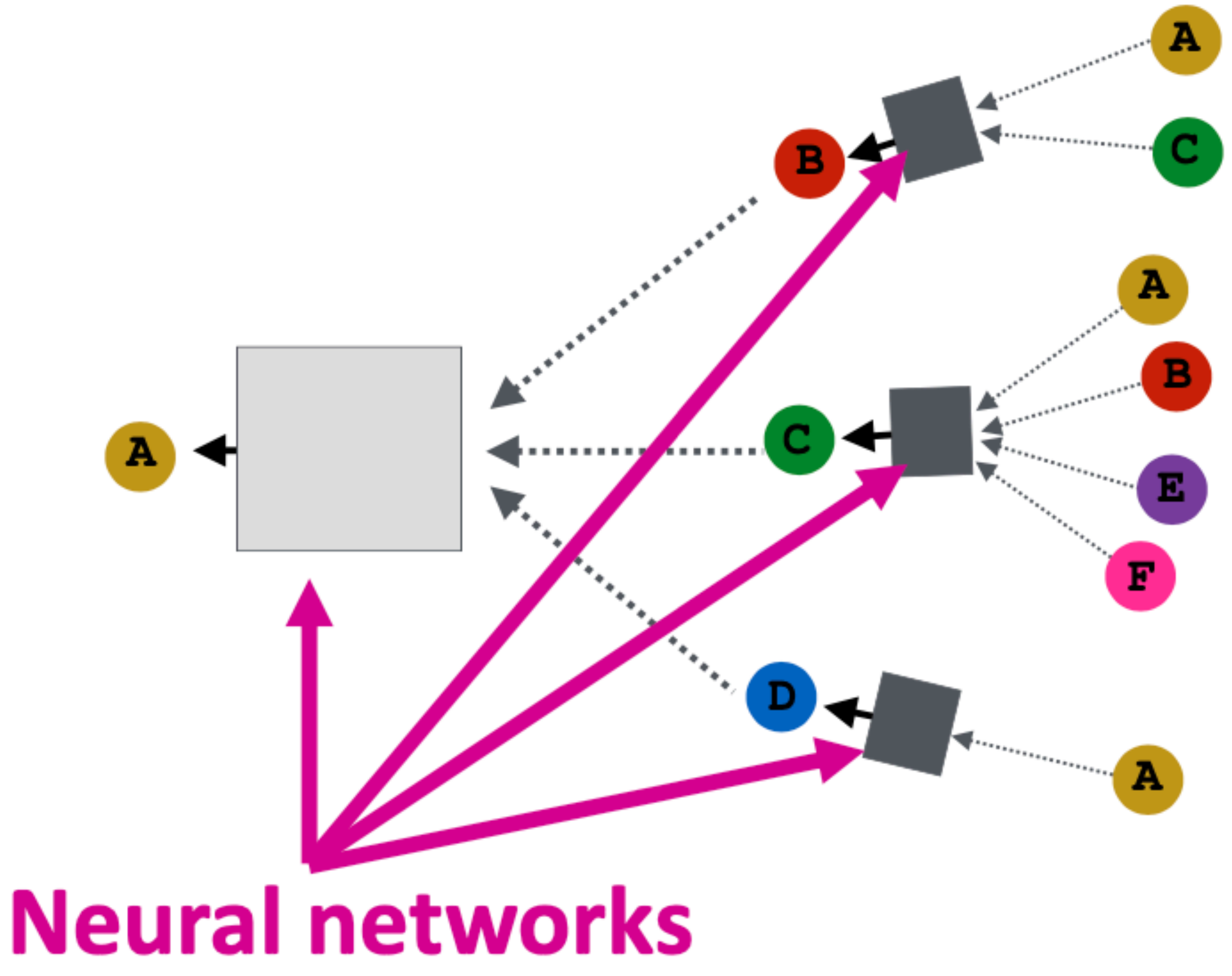
GraphSAGE = **Graph** + **SA**mple + aggre**G**at**E**

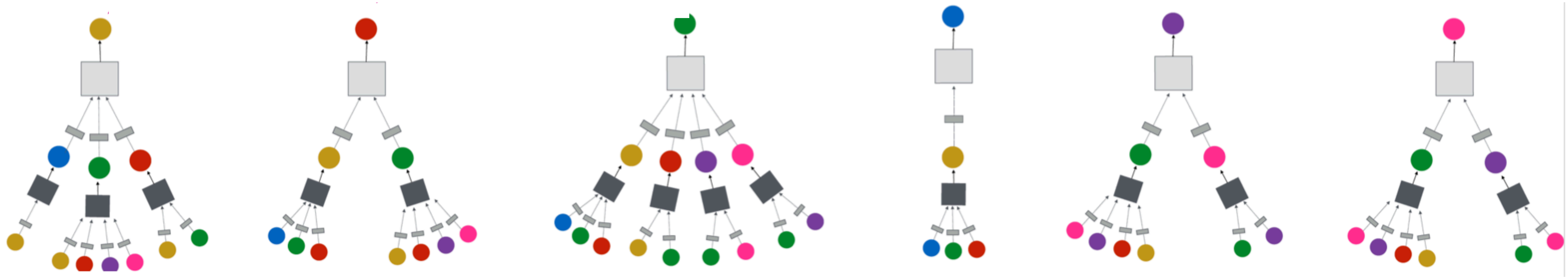


Generate node embeddings based on local network neighborhoods

GraphSAGE: Aggregate







Layer K = 2

GraphSAGE : Aggregator Architectures

Invariant to permutations of its input(no nature **ordering**)

- **Mean**

$$\mathbf{h}_v^k \leftarrow \sigma\left(\mathbf{W}^k \cdot \text{MEAN}\left(\{\mathbf{h}_v^{k-1}\} \cup \{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\}\right)\right)$$

- **LSTM**

Adapt LSTMs to operate on an unordered set by simply applying the LSTMs to a random permutation of the node's neighbor

- **Pooling**

$$\text{AGREGATE}_k^{\text{pool}} = \max\left(\left\{\sigma\left(\mathbf{W}_{\text{pool}}\mathbf{h}_{u_i}^k + \mathbf{b}\right), \forall u_i \in \mathcal{N}(v)\right\}\right)$$

GraphSAGE : Parameters

$$\mathbf{h}_v^k = \sigma\left(\left[\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|}, \mathbf{B}_k \mathbf{h}_v^{k-1}\right]\right), \forall k \in \{1, \ldots, K\} \tag{1}$$

Weight matrices and parameters of the aggregator functions

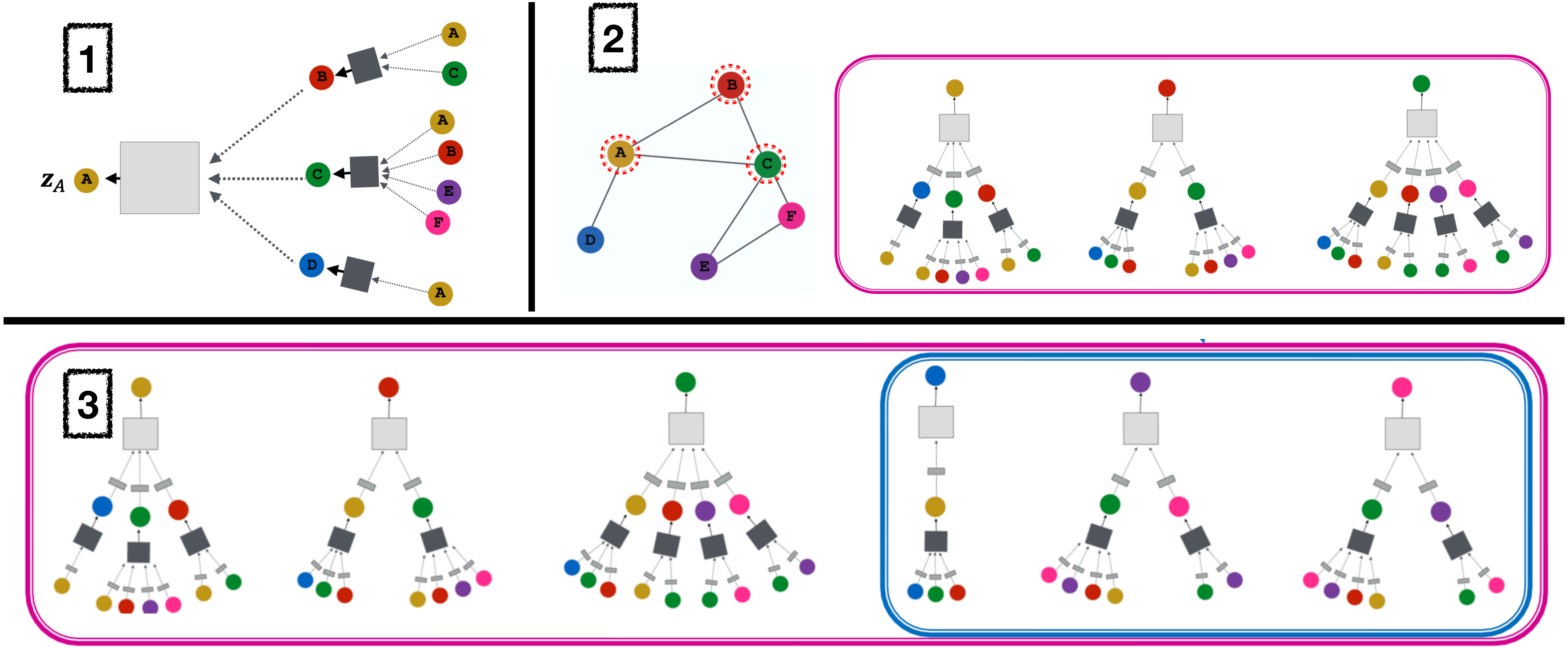
Unsupervised

$$J_{\mathcal{G}}\left(\mathbf{z}_u\right) = -\log\left(\sigma\left(\mathbf{z}_u^\top \mathbf{z}_v\right)\right) - Q \cdot \mathbb{E}_{v_n \sim P_n(v)} \log\left(\sigma\left(-\mathbf{z}_u^\top \mathbf{z}_{v_n}\right)\right) \tag{2}$$

Supervised

$$\mathscr{L}\left(h_A\right) = ||y_A - f\left(h_A\right)||^2 \tag{3}$$

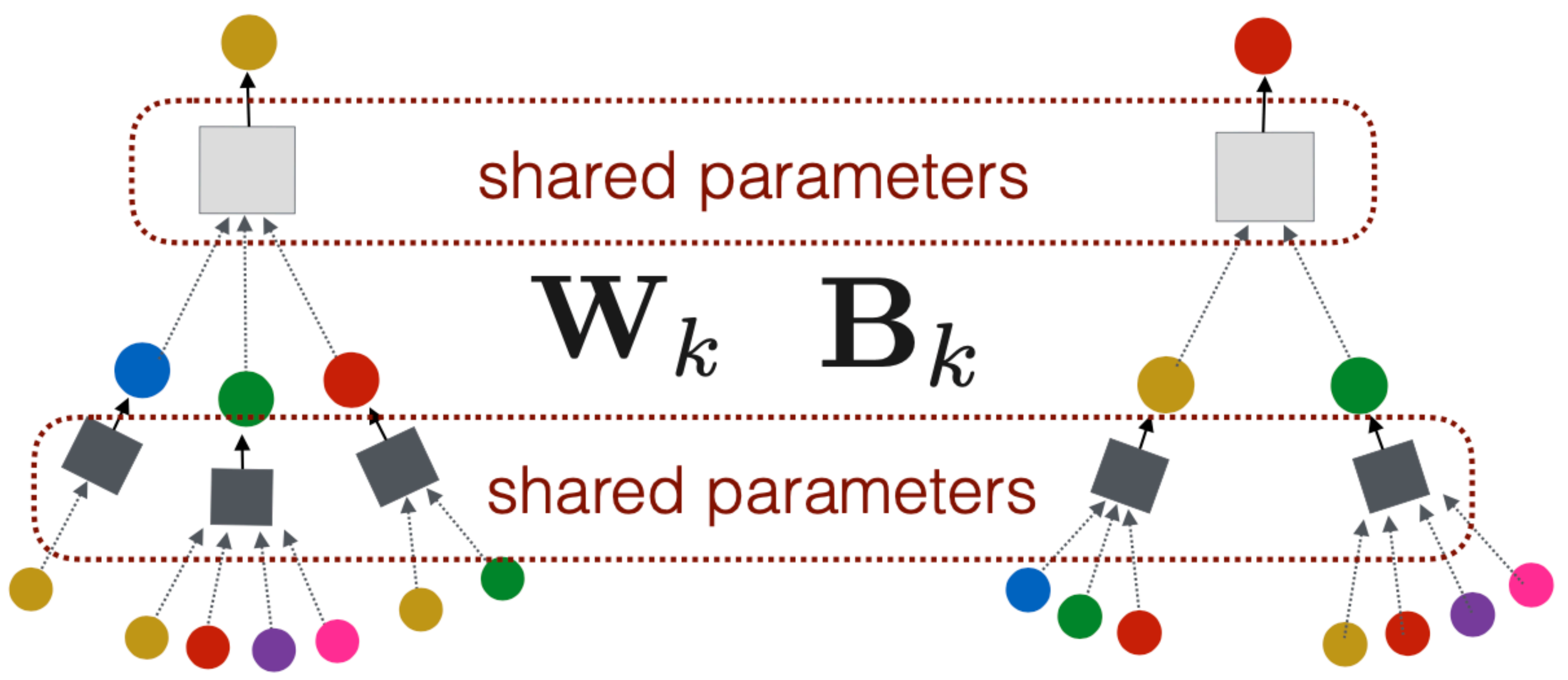
GraphSAGE : Overview



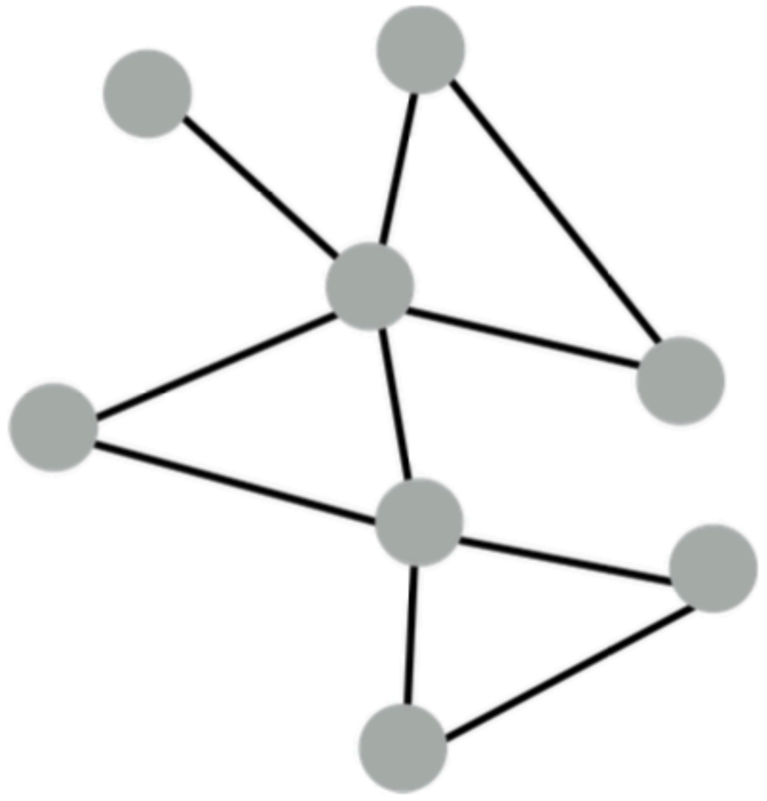
1. *Define a neighborhood aggregation function and a loss function on the embeddings*
2. *Train on a set of nodes, i.e., a batch of compute graphs*
3. *Generate embeddings for nodes as needed(Even for nodes we never trained on)*

GraphSAGE : Inductive

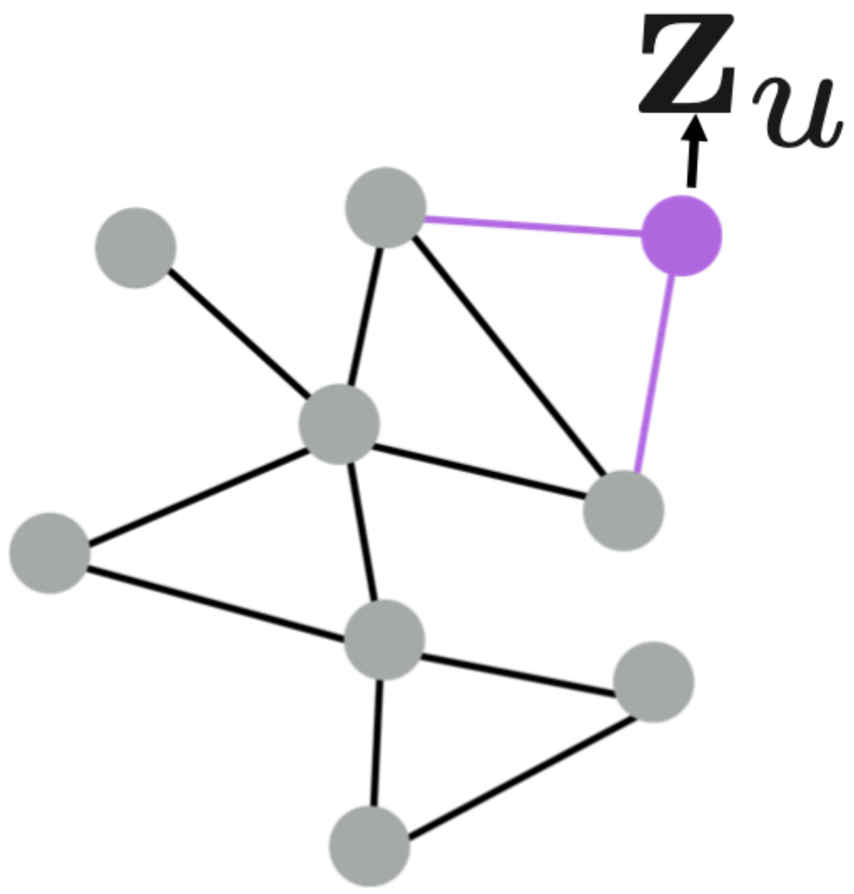
The same aggregation parameters
are shared for all nodes



New node

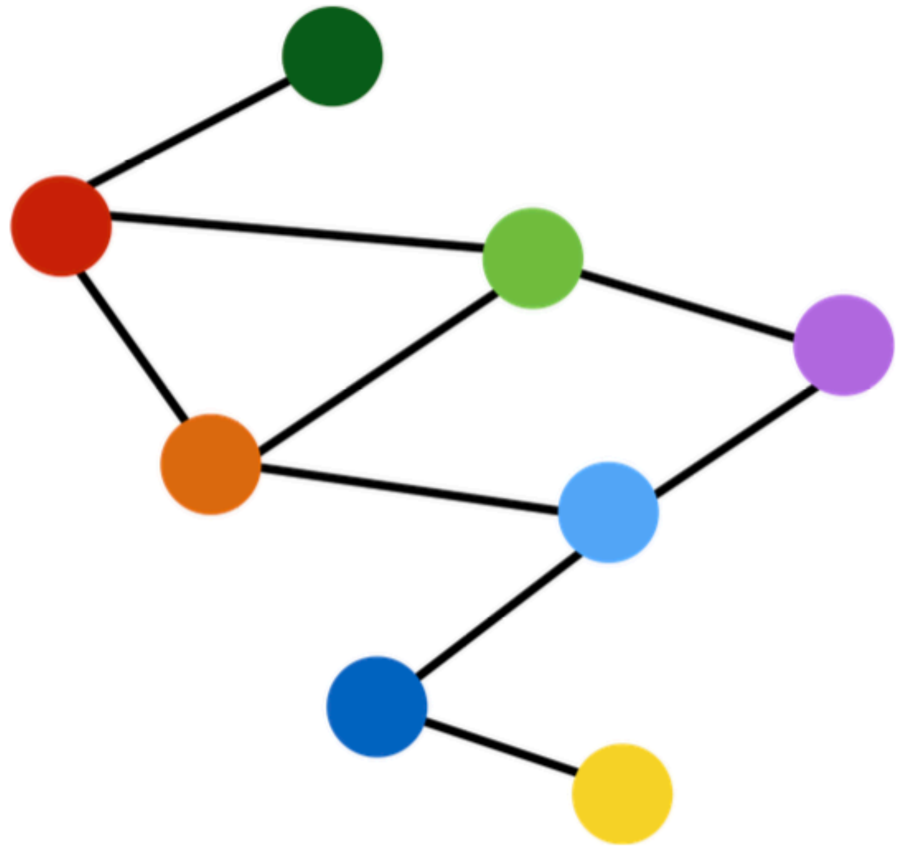


Train graph

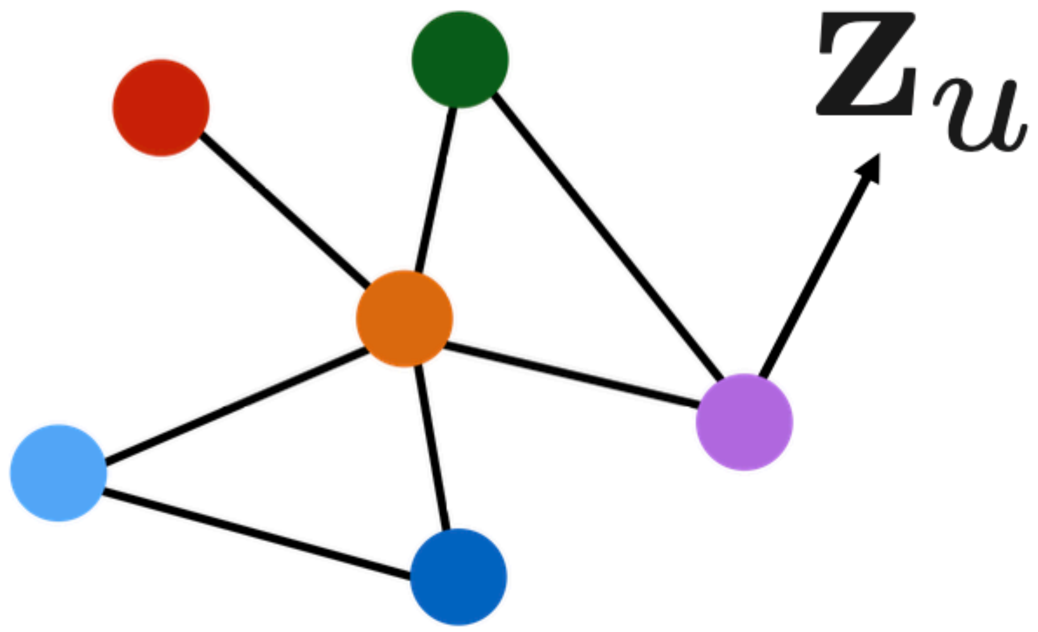


Generate embedding
for new node

New graph



Train graph



Generalize to new graph

Experiments

Set-up :

- Test the performance on **node-classification task.**
- Evaluation on three datasets : Citation, Reddit, PPI.
- For all the GraphSAGE, set $K = 2$,with neighborhood **sample sizes** $S_1 = 25$ and $S_2 = 10$.

Baselines :

- **Random :** a random classifier.
- **Logistic:** a logistic regression feature-based classifier.
- **DeepWalk :** a representative factorization-based approach.

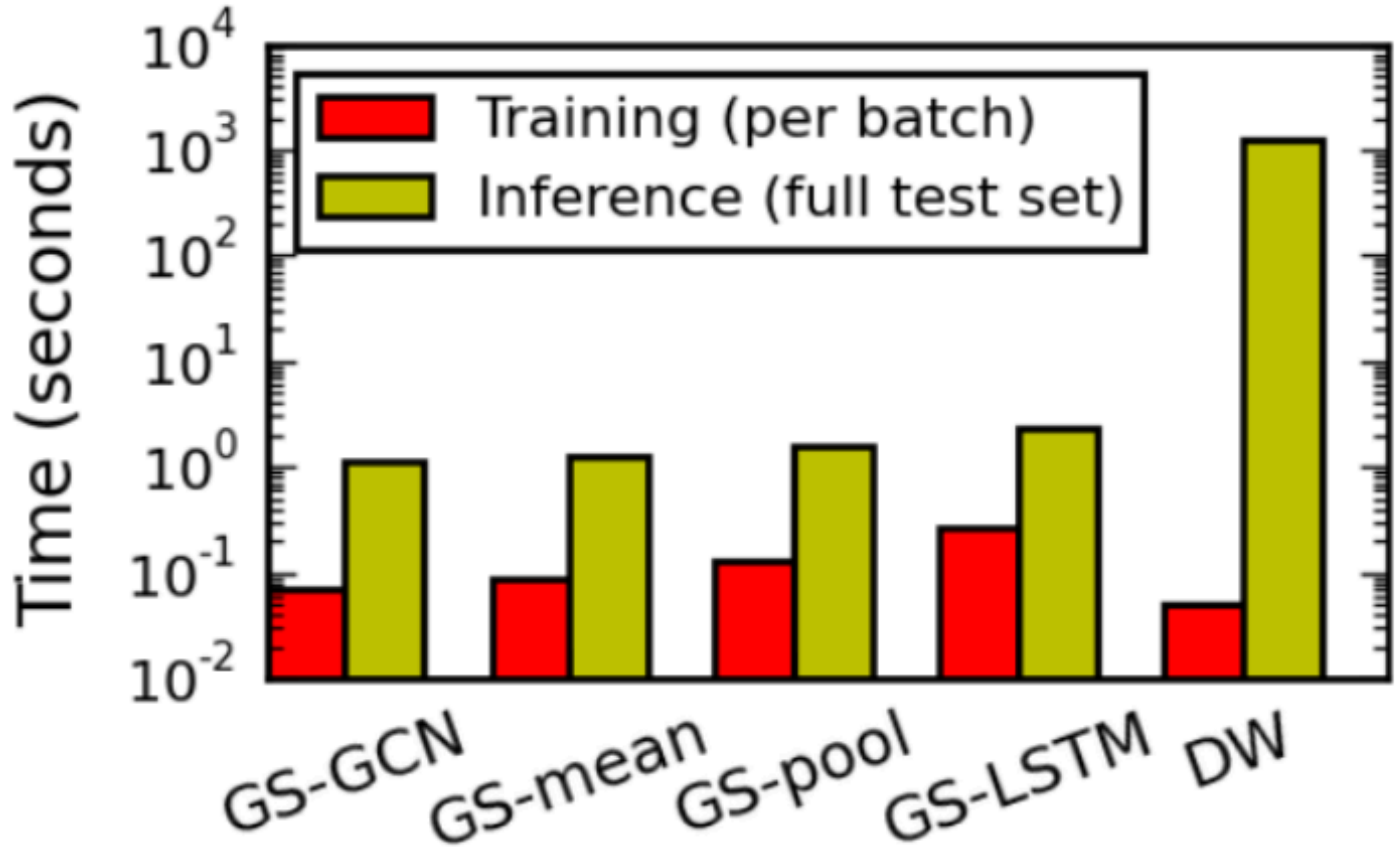
Results

Name	Citation Unsup. F1	Citation Sup. F1	Reddit Unsup. F1	Reddit Sup. F1	PPI Unsup. F1	PPI Sup. F1
Random	0.206	0.206	0.043	0.042	0.396	0.396
Raw features	0.575	0.575	0.585	0.585	0.422	0.422
DeepWalk	0.565	0.565	0.324	0.324	—	—
DeepWalk + features	0.701	0.701	0.691	0.691	—	—
GraphSAGE-GCN	0.742	0.772	**0.908**	0.930	0.465	0.500
GraphSAGE-mean	0.778	0.820	0.897	0.950	0.486	0.598
GraphSAGE-LSTM	0.788	0.832	**0.907**	**0.954**	0.482	**0.612**
GraphSAGE-pool	**0.798**	**0.839**	0.892	0.948	**0.502**	0.600
% gain over feat.	39%	46%	55%	63%	19%	45%

GraphSAGE significantly outperforms the baseline approaches

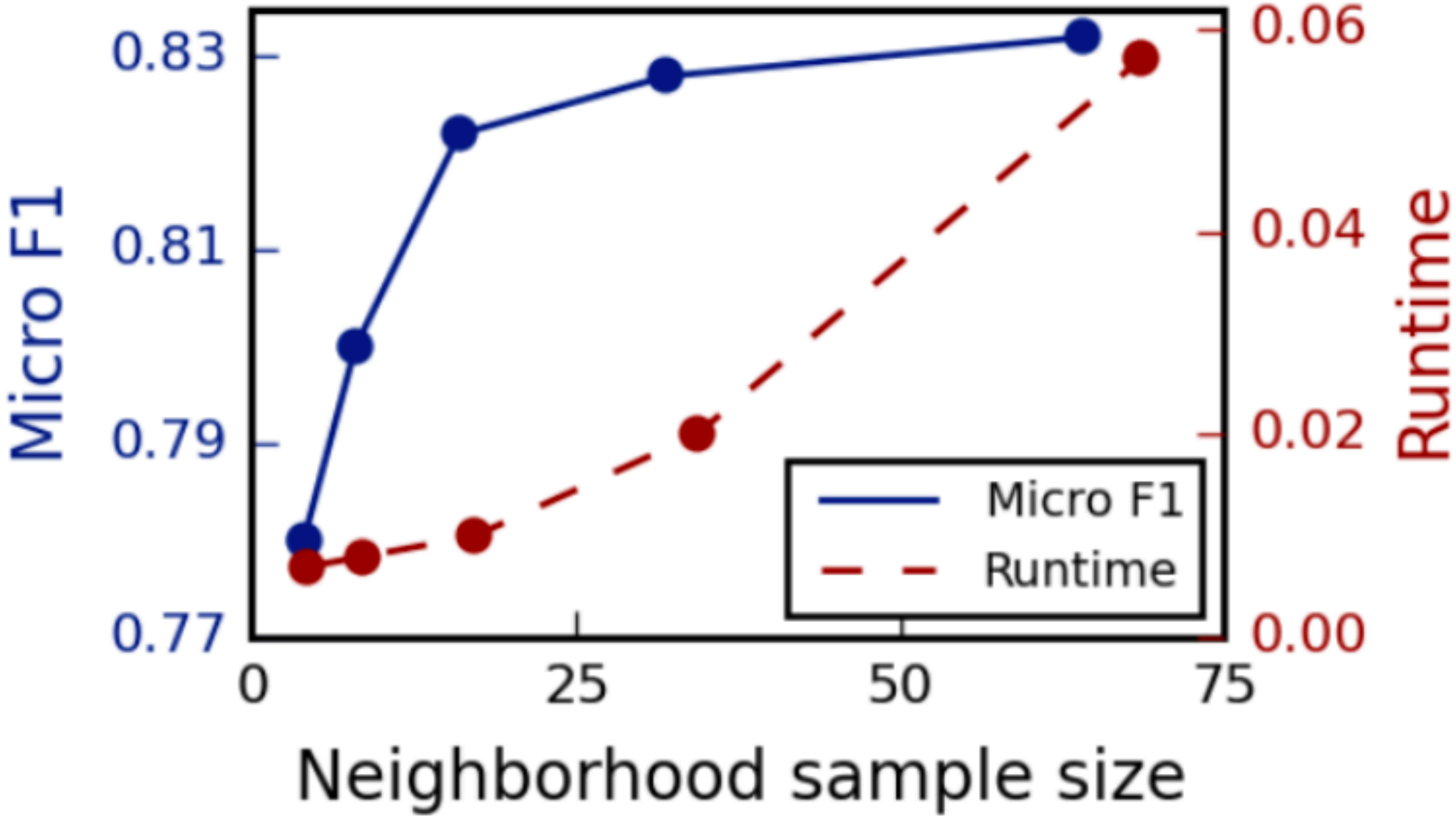
Results

Timing experiments



DeepWalk 100-500× slower at test time

Size of the sampled neighborhood



K = 2 with S1 = S2

Analyze

- ☑ A "**deep**" model rather than traditional "shallow" model(eg. DeepWalk).
- ☑ Leverages both node **feature information** and graph structure rather than only graph structure.
- ☑ An **inductive** model rather than a transduction model.
- ☑ Apply on **large** graphs(eg. 10 billion nodes).

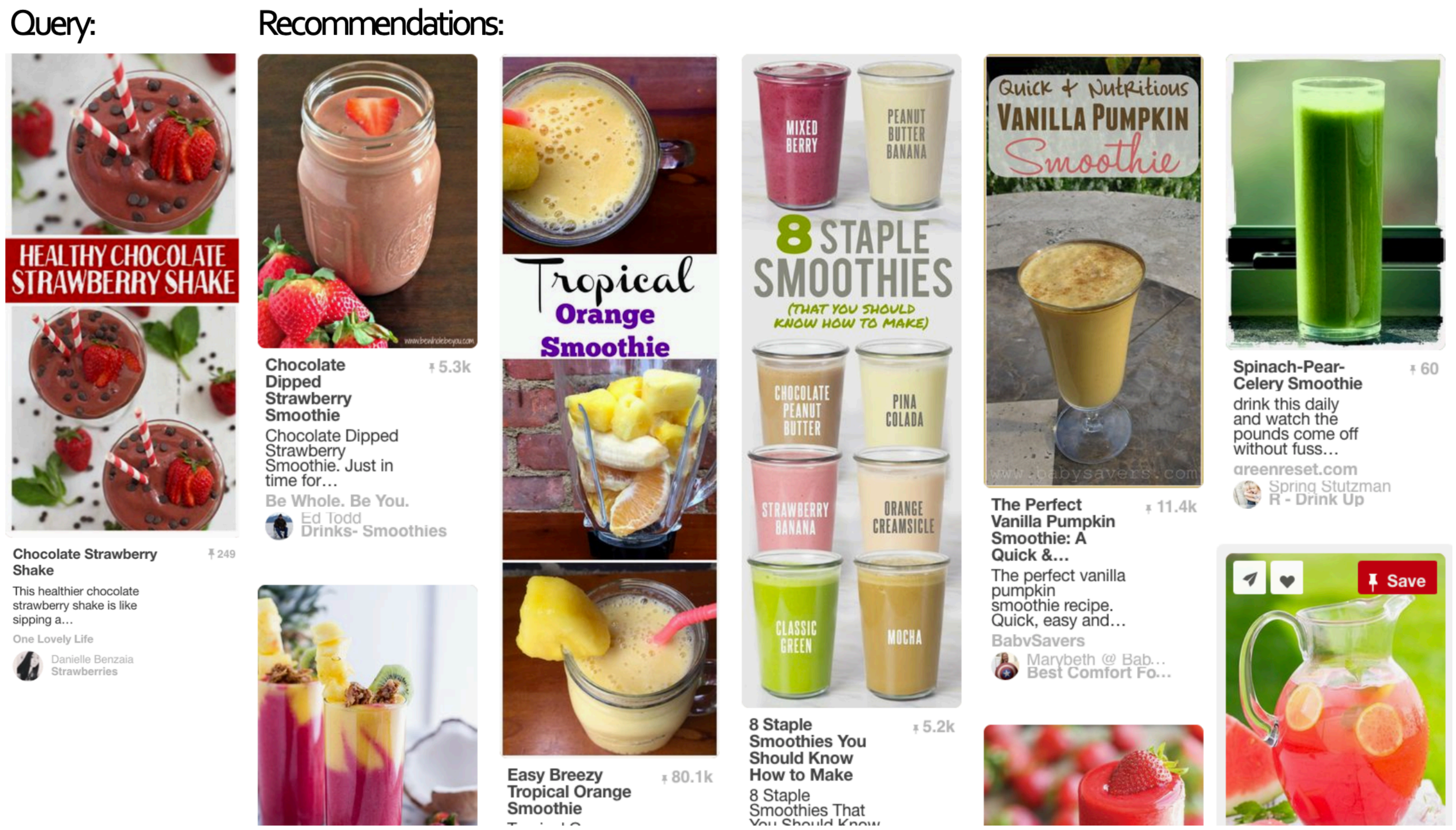
- ☐ Can't learn on **directed** or **multi-modal** graphs.
- ☐ Use a **uniform** neighborhood sampling functions.
- ☐ Apply the **same weights** to different neighborhoods.

Conclusion

- Present GraphSAGE to solve representation of nodes on large graphs.
- It's a general inductive framework that leverages node feature information and graph structure.
- It outperforms strong baselines on three node-classification benchmark.

https://github.com/williamleif/GraphSAGE

Application : PinSAGE

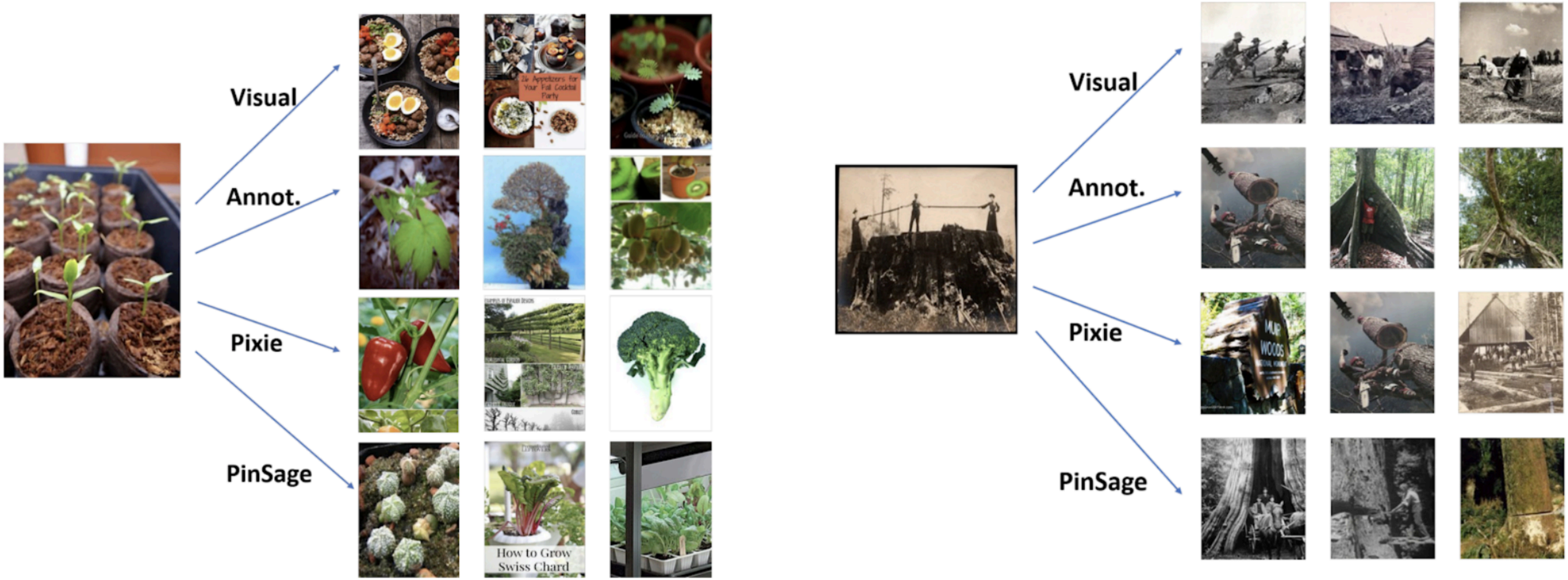


Pinterest + Stanford

3 billion nodes representing pins and boards, and 18 billion edges

Graph Convolutional Neural Networks for Web-Scale Recommender Systems , Jure Leskovec, 2018 KDD

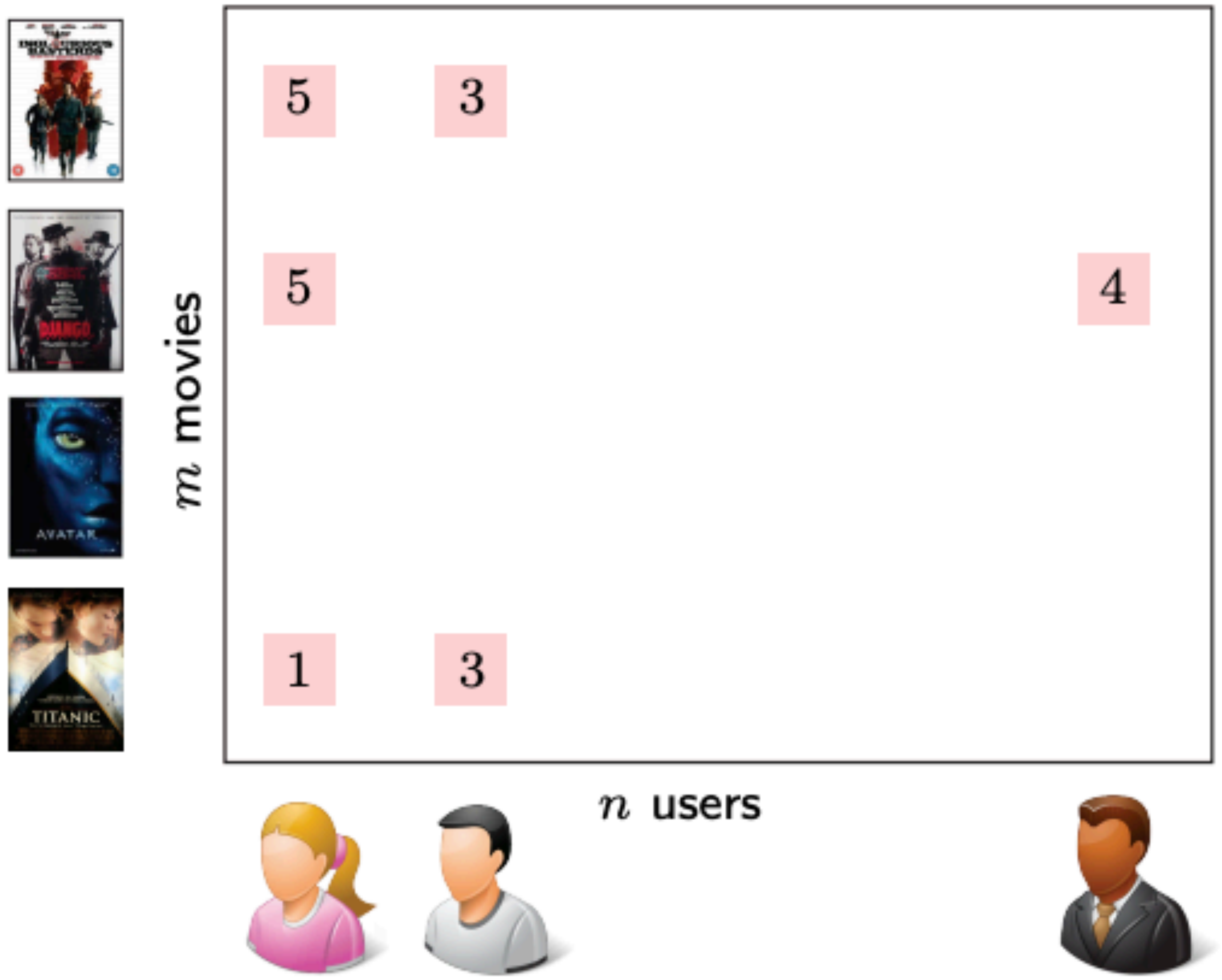
Application : PinSAGE

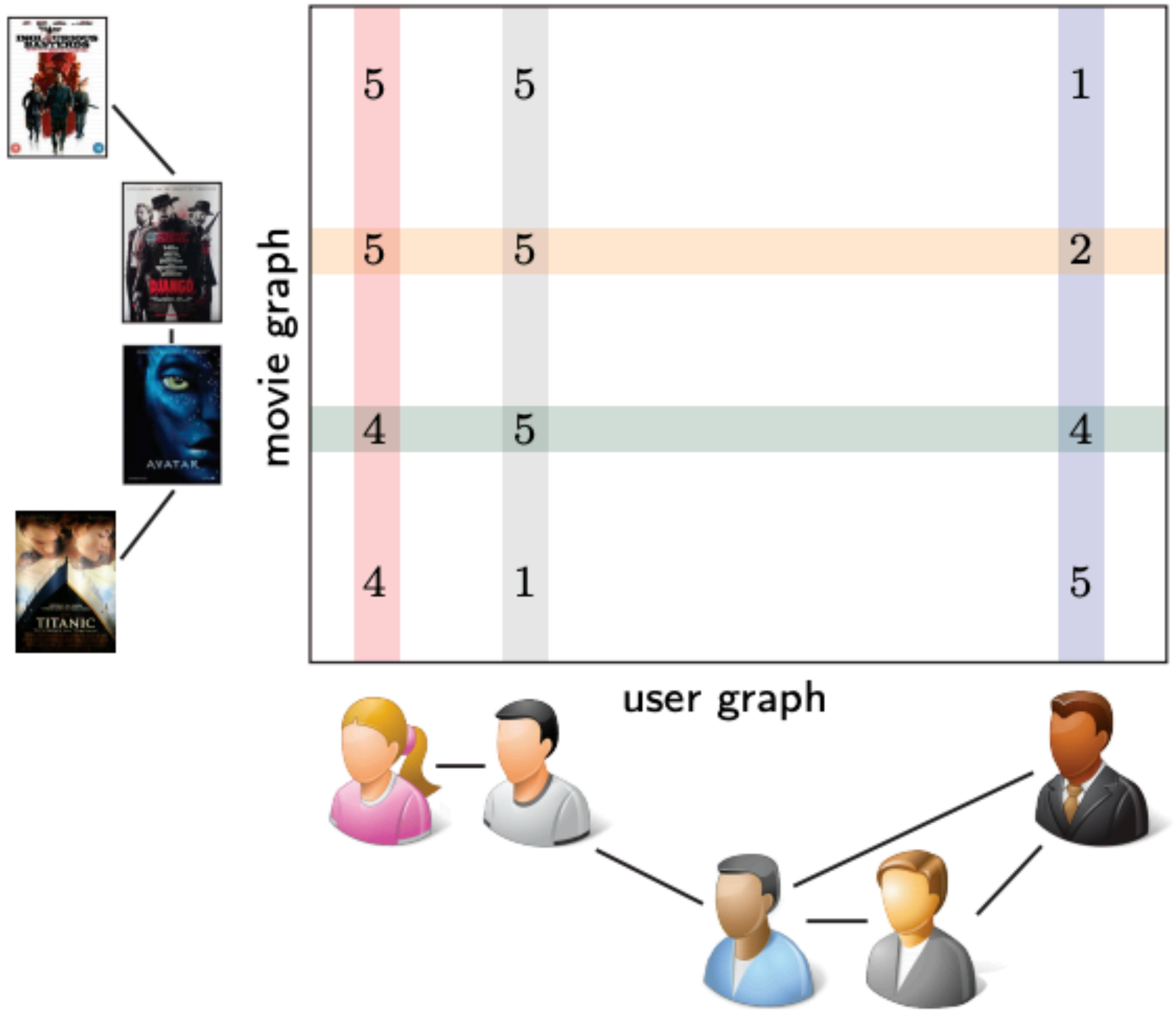


Graph Convolutional Neural Networks for Web-Scale Recommender Systems,Jure Leskovec, 2018 KDD

Application

Recommender System





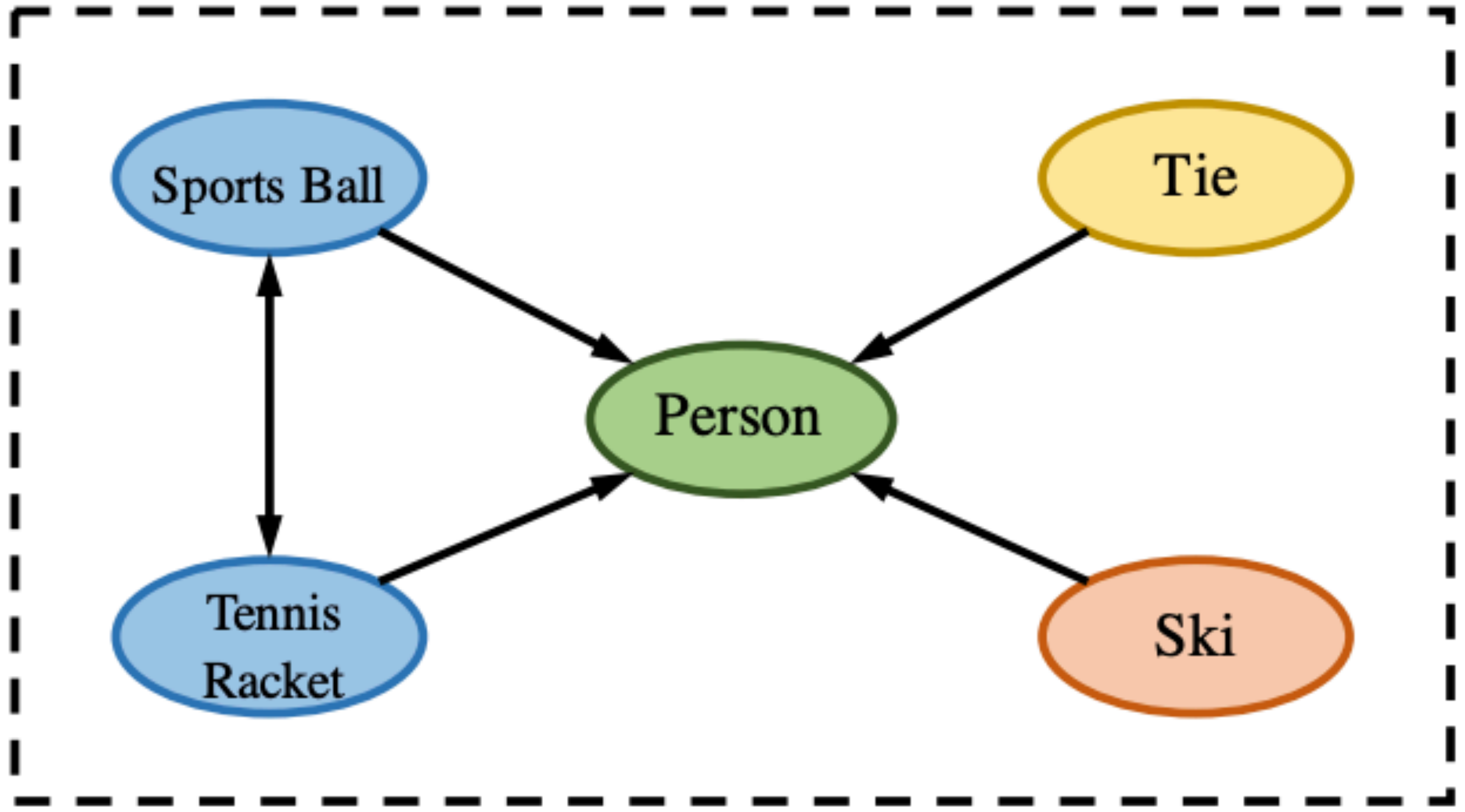
Application

Multi-Label Image Recognition

Person, Sports Ball, Tennis Racket

Person, Tie

Person, Ski



Multi-Label Image Recognition with Graph Convolutional Networks, Zhao-Min Chen, CVPR 2019

Application

3. Applications	
3.1 Physics	3.2 Chemistry and Biology
3.3 Knowledge Graph	3.4 Recommender Systems
3.5 Computer Vision	3.6 Natural Language Processing
3.7 Generation	3.8 Combinatorial Optimization
3.9 Adversarial Attack	3.10 Graph Clustering
3.11 Graph Classification	3.12 Reinforcement Learning
3.13 Traffic Network	3.14 Few-shot and Zero-shot Learning
3.15 Program Representation	3.16 Social Network

https://github.com/thunlp/GNNPapers