Machine Learning on graphs. Graph Neural Networks

I. Makarov & L.E. Zhukov

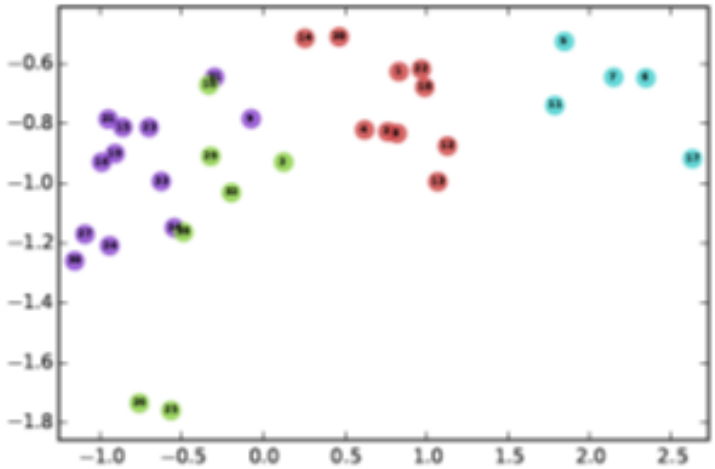
BigData Academy MADE from VK

Network Science

Lecture outline

Graph Embeddings

- Necessity to automatically select features
- Reduce domain- and task- specific bias
- Unified framework to vectorize network
- Preserve graph properties in vector space
- Similar nodes $\rightarrow$ close embeddings

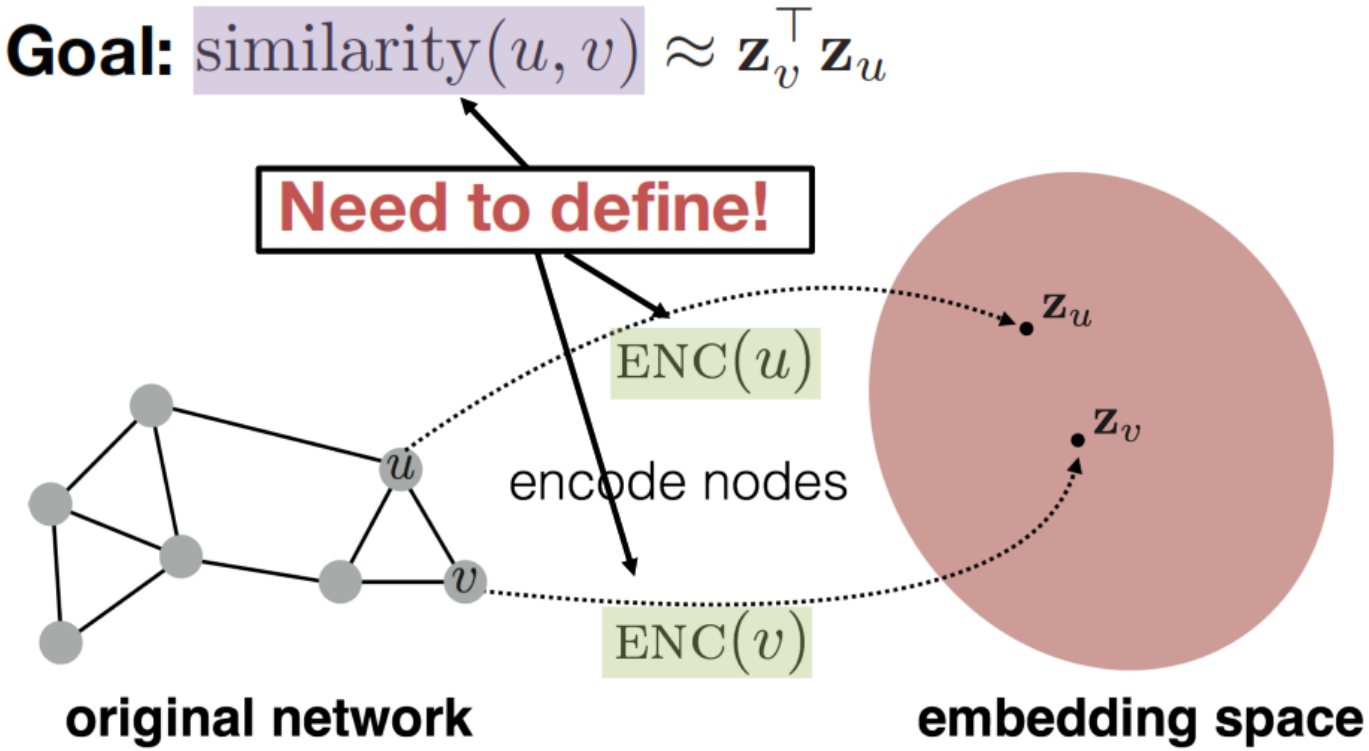


from Leskovec et al., 2018[1]

[1] http://snap.stanford.edu/proj/embeddings-www/

Graph Embeddings

- Define **Encoder**
- Define **Similarity**/graph feature to preserve graph properties
- Define similarity/distance in the embedding space
- **Optimize** loss to fit embedding with similarity computed on graph



from Leskovec et al., 2018

Random Walks

- Similarity between u and v is probability to co-occur on a random walk
- Sample each vertex u neighborhood $N_R(u)$ (multiset) by short random walks via strategy R
- Optimize similarity considering independent neighbor samples via MLE (remind Word2Vec)

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$$

from Leskovec et al., 2018

Short conclusion for structural Graph Embeddings

- Random walks are powerfull tool for fast network embedding
- Proximity-aware embeddings, random walks can be modelled in terms of each other (and even deep neural networks !)
- complexity and space are important to choose the embedding model
- provided models are used for transductive learning only, inductive learning require additional regularizations and local optimizations
- large graphs are hard to fit with handcrafted sampling strategies
- no clear way to support features

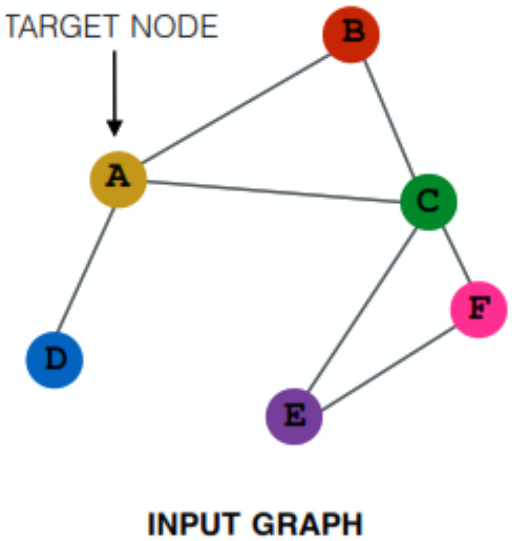
GNN

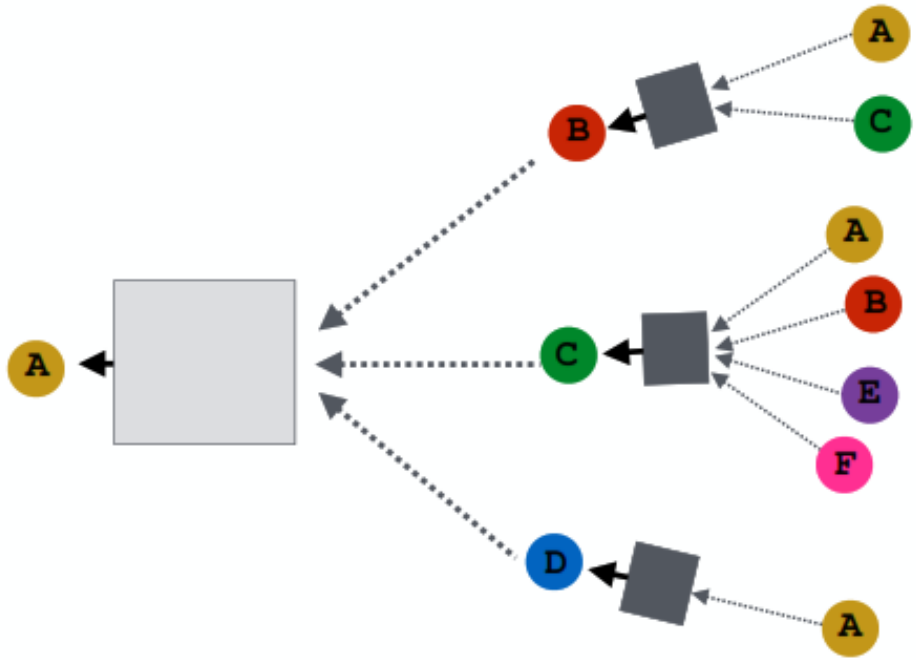
Graph Neural Network: Setting

- We have a graph $G(V, E)$ defined by adjacency matrix A and feature matrix $X \in \mathrm{R}^{f,|V|}$
- Confirmed relation between closeness of feature space and graph structure
- Non-graph features are vectorized separately (images, texts, one-hot encoding for labels, numeric features)

Graph Neural Network: Idea

- Assign weights only to information obtained from neighbors
- Include node itself via loop with trainable weight
- Each node generate its own computational graph

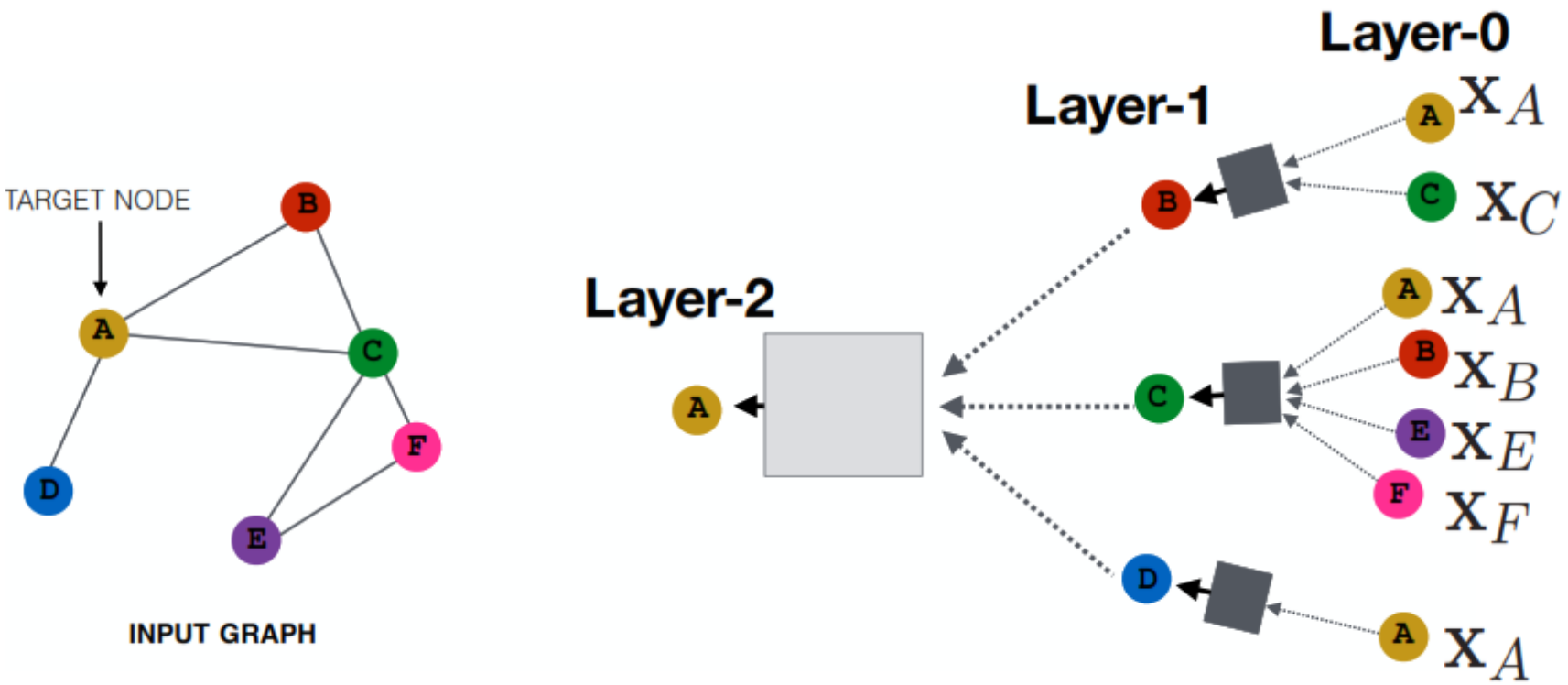




from Leskovec et al., 2018

Graph Neural Network: Layer structure

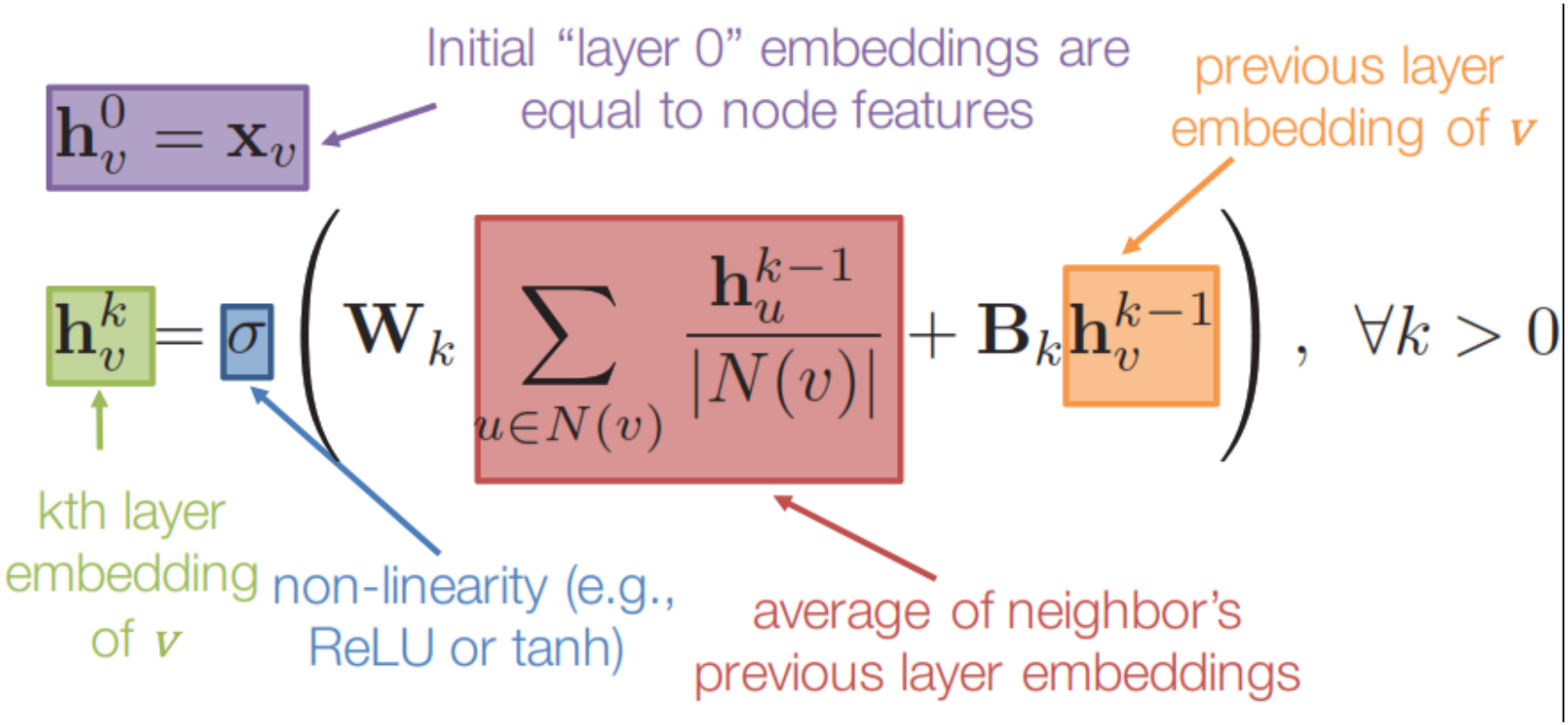
- Each aggregation defines new layer
- Zero-level embedding is non-graph feature
- Arbitrary depth but remember on "law of six handshakes"



from Leskovec et al., 2018

Graph Neural Network: Basic Approach

- Aggregation over weighted sum of neighbor input and node itself under non-linearity
- Use simple neural network construction



from Leskovec et al., 2018

Graph Neural Network: Training

- Stop at K-th layer and feed h_v^K as embeddings to task-dependent loss; use SGD to optimize
- Unsupervised training uses reconstruction loss of adjacency matrix A (MSE, CE)
- (Semi-)Supervised loss feeds node embeddings to FC layer to predict labels under CE loss with possible Laplacian regularization
- When no features available, unsupervised training uses either one hot encoding for nodes (each node - separate label), or pretrains some structural embedding and feed them into feature matrix

Graph Neural Network: General Pipeline

- Define Aggregator
  - Different aggregators support only transductive learning for static graph
  - Sharing layer-wise weights allows inductive learning and inference on unseen nodes
- Define Loss
- Train on batches of nodes
- Generate output embeddings

GCN

Graph Convolutional Network

- Aggregation over shared weights between node and its neighbors
- Normalization to stabilize training for high-degree nodes

Basic Neighborhood Aggregation

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right)$$

VS.

GCN Neighborhood Aggregation

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v) \cup v} \frac{\mathbf{h}_u^{k-1}}{\sqrt{|N(u)||N(v)|}}\right)$$

same matrix for self and neighbor embeddings

per-neighbor normalization

from Leskovec et al., 2018

Graph Convolutional Network

- Efficient batch computation in matrix form
- Obtained $O(|\ E\ |)$ complexity (see pyG, DGL libraries)

$$\mathbf{H}^{(k+1)} = \sigma\left(\mathbf{D}^{-\frac{1}{2}}\tilde{\mathbf{A}}\mathbf{D}^{-\frac{1}{2}}\mathbf{H}^{(k)}\mathbf{W}_k\right)$$

$$\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$$

$$\mathbf{D}_{ii} = \sum_j \mathbf{A}_{i,j}$$

from Leskovec et al., 2018

GAT

Graph ATtention Network

- Not all the neighbors are equal

$$e_{ij} = a(\mathbf{W}\vec{h}_i, \mathbf{W}\vec{h}_j)$$

$$\alpha_{ij} = \text{softmax}_j(e_{ij}) = \frac{\exp(e_{ij})}{\sum_{k \in \mathcal{N}_i} \exp(e_{ik})}$$

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k \in \mathcal{N}_i} \exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k]\right)\right)}$$

$\|$ is the concatenation operation.

$$\vec{h}'_i = \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \mathbf{W}\vec{h}_j\right)$$

from Bengo et al., 2018

Graph ATtention Network

- Multi-head attention works better like in different convolution filters
- Final layer require pooling isntead of concatenation

$$\vec{h}'_i = \sigma\left(\sum_{j\in\mathcal{N}_i} \alpha_{ij}\mathbf{W}\vec{h}_j\right)$$

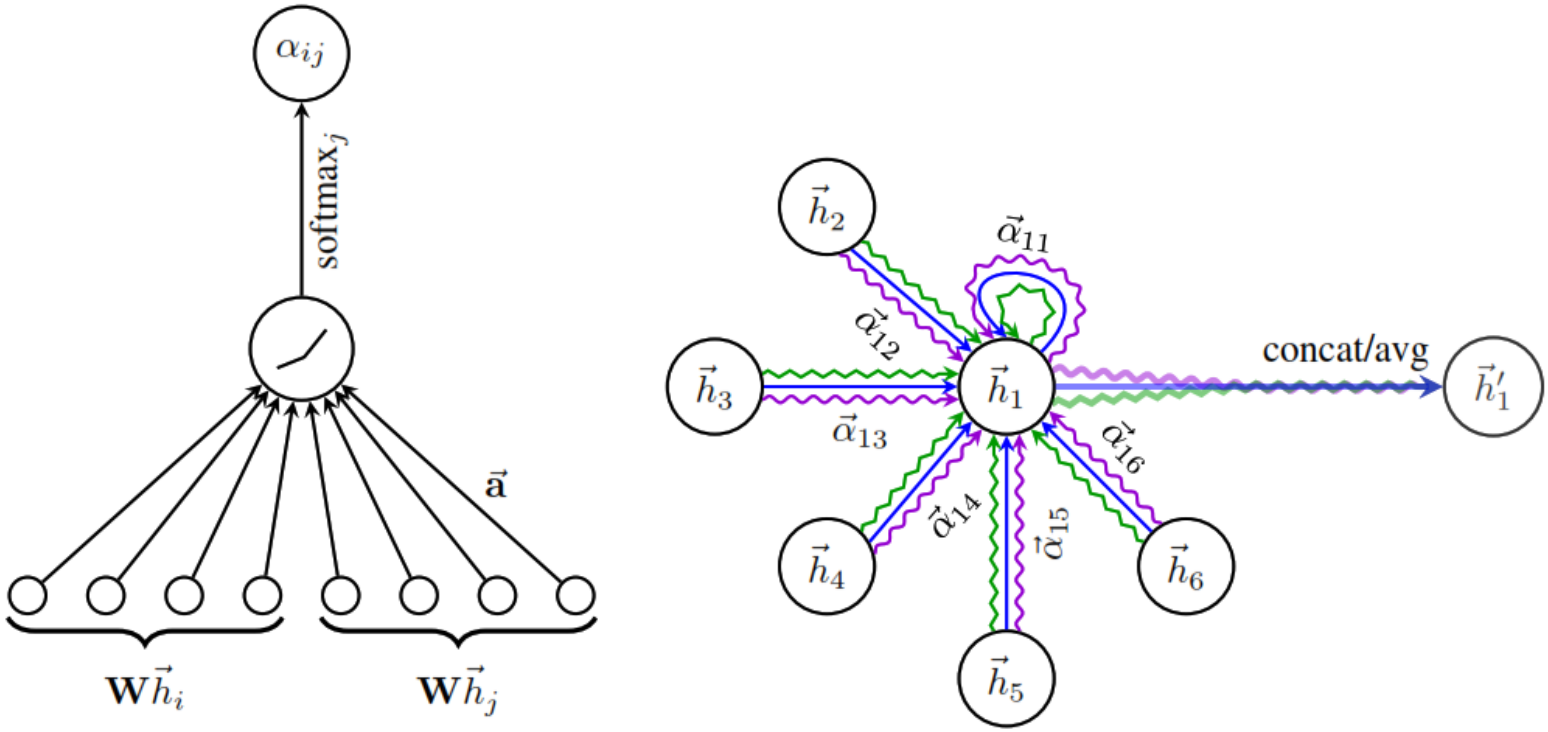
$$\vec{h}'_i = \Big\Vert_{k=1}^{K} \sigma\left(\sum_{j\in\mathcal{N}_i} \alpha_{ij}^k\mathbf{W}^k\vec{h}_j\right)$$

$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i} \alpha_{ij}^k\mathbf{W}^k\vec{h}_j\right)$$

from Bengo et al., 2018

Graph ATtention Network

- Feature aggregation via attention over learned weights
- Different patterns for the same structure



from Bengo et al., 2018

GraphSAGE

GraphSAGE: Feature Pyramid

- Vary feature space across layers
- Aggregate from neighbors and concatenate with self-representation

Simple neighborhood aggregation:

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right)$$

GraphSAGE:

concatenate self embedding and neighbor embedding

$$\mathbf{h}_v^k = \sigma\left(\left[\mathbf{W}_k \cdot \mathrm{AGG}\left(\{\mathbf{h}_u^{k-1}, \forall u \in N(v)\}\right), \mathbf{B}_k \mathbf{h}_v^{k-1}\right]\right)$$

generalized aggregation

from Leskovec et al., 2018

GraphSAGE: Differentiable Aggregators

Mean:

$$\text{AGG} = \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|}$$

Pool

element-wise mean/max

$$\text{AGG} = \gamma\left(\{\mathbf{Q}\mathbf{h}_u^{k-1}, \forall u \in N(v)\}\right)$$

LSTM:

- Apply LSTM to random permutation of neighbors.

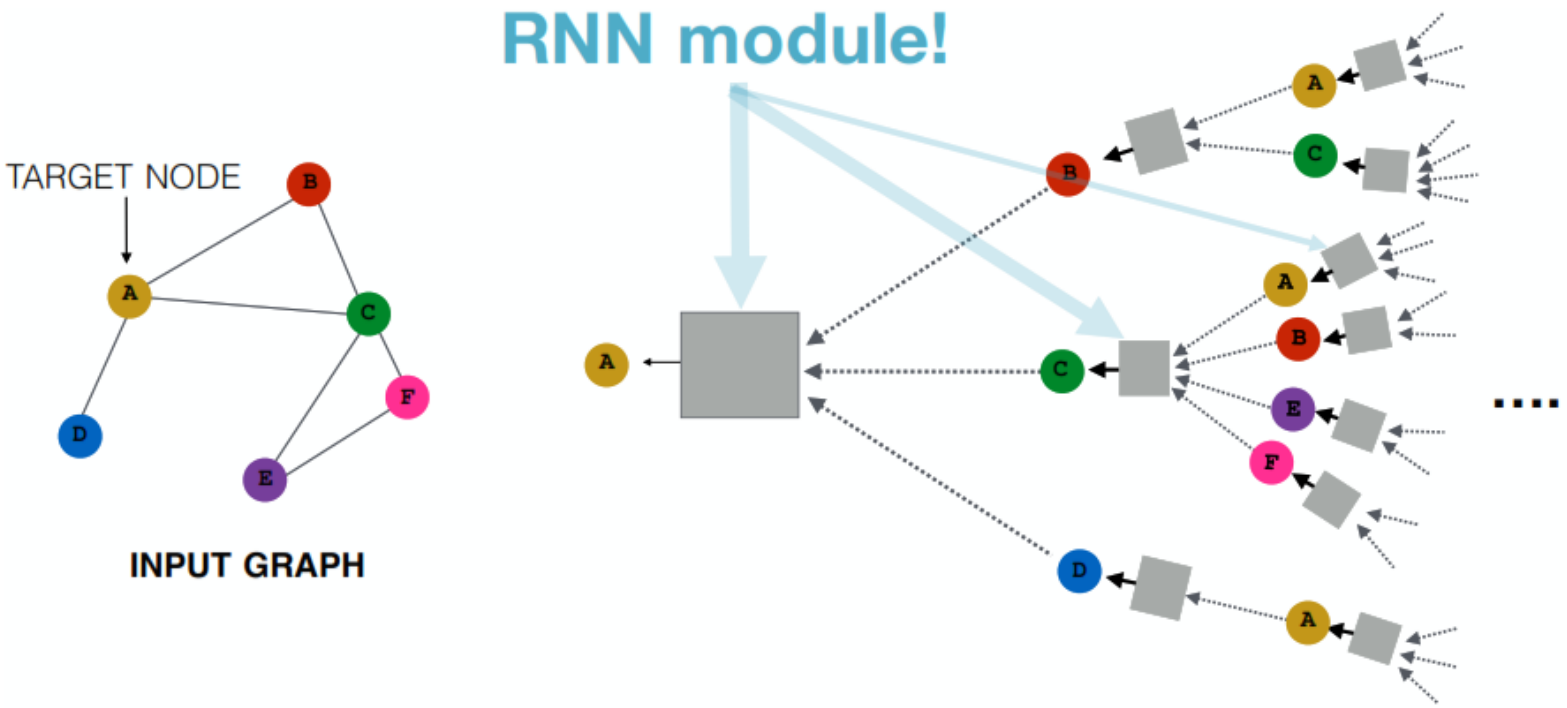
$$\text{AGG} = \text{LSTM}\left([\mathbf{h}_u^{k-1}, \forall u \in \pi(N(v))]\right)$$

from Leskovec et al., 2018

How to fight dimension curse

Model Depth

- Usually 2-3 layers for GCN / GraphSAGE
- More layers make method global
- Computation graph exceed memory limits
- Overfitting, vanishing gradient



from Leskovec et al., 2018

Gated GNN

- Use recurrent model with shared weights across all the layers, support any depth

1. Get "message" from neighbors at step k:

$$\mathbf{m}_v^k = \mathbf{W} \sum_{u \in N(v)} \mathbf{h}_u^{k-1}$$

aggregation function does not depend on k

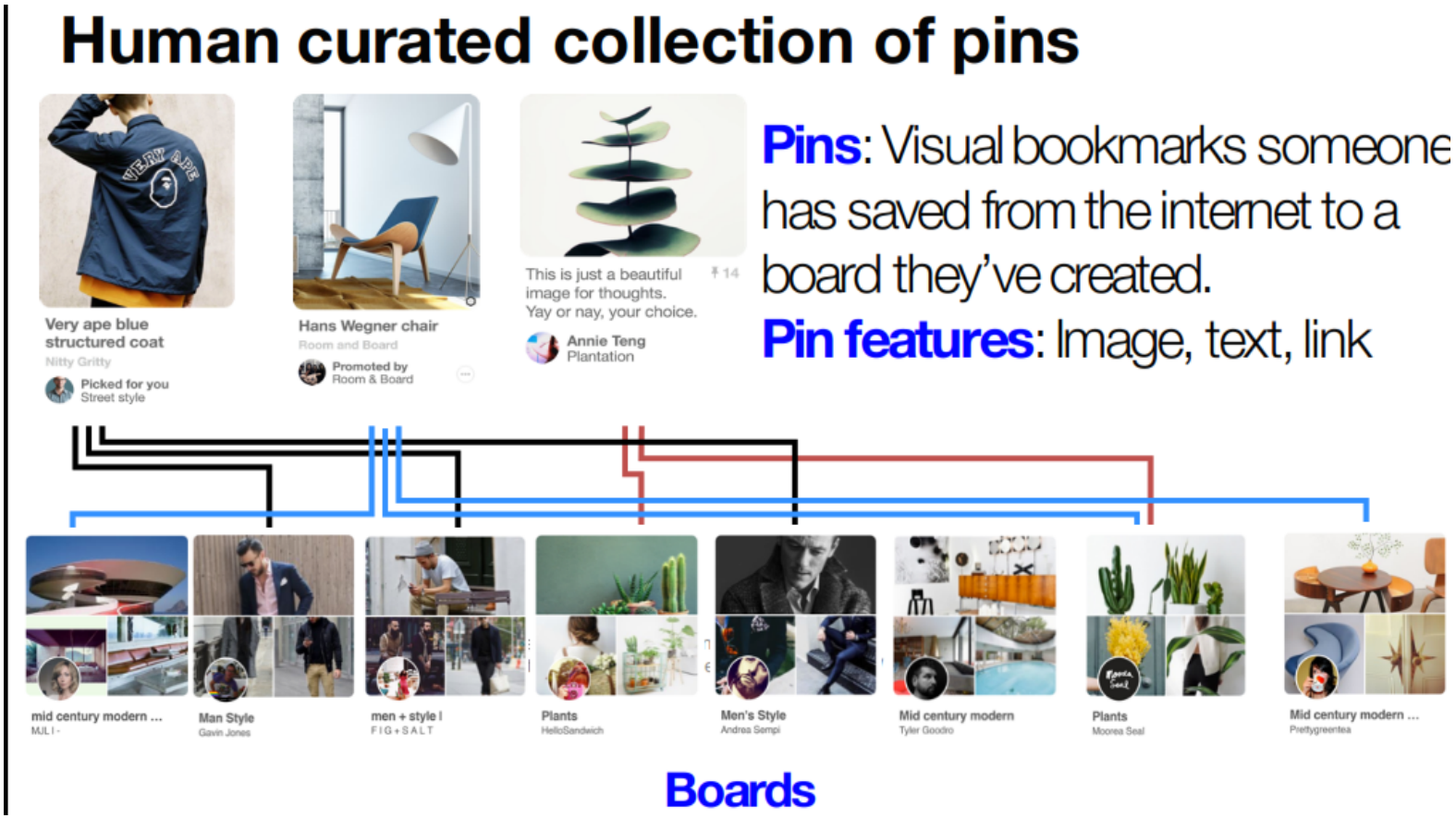
2. Update node "state" using Gated Recurrent Unit (GRU). New node state depends on the old state and the message from neighbors:

$$\mathbf{h}_v^k = \mathrm{GRU}(\mathbf{h}_v^{k-1}, \mathbf{m}_v^k)$$

from Leskovec et al., 2018

Large Scale RecSys: PinSAGE

- Pinterest: 3 billion pins and boards; 16 billion interactions; label, text and image features



from Leskovec et al., 2018

Large Scale RecSys: PinSAGE

Recommendations pipeline:

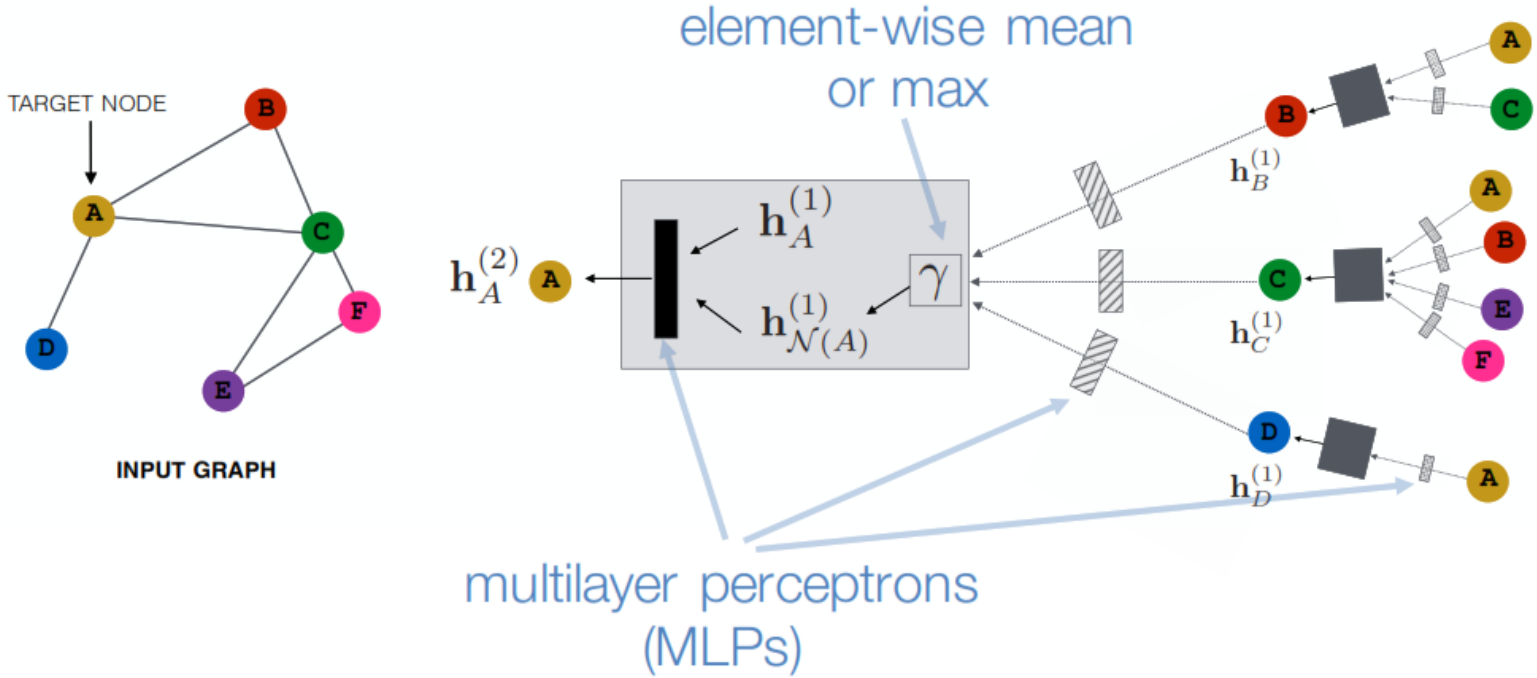
- Collect consequent clicks
- Train system using metric learning approach
- Generate embeddings
- Recommend via k-NN

Key advances:

- Sub-sample neighborhoods for efficient GPU batching
- Producer-consumer training pipeline
- Curriculum learning for negative samples
- MapReduce for efficient inference

Large Scale RecSys: RW-GCN

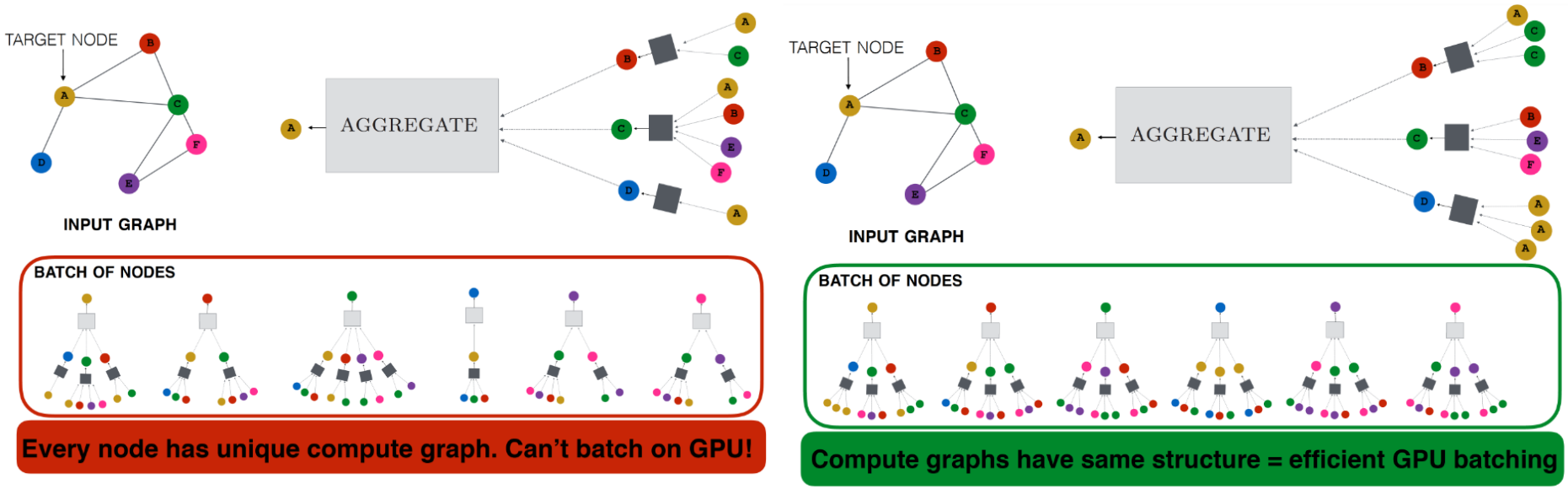
- Train so that pins that are consecutively clicked have similar embeddings, use smart negative sampling



from Leskovec et al., 2018

Large Scale RecSys: Batch Sampling

- Use one computation graph, sample nodes according top-PPR among neighbors



from Leskovec et al., 2018

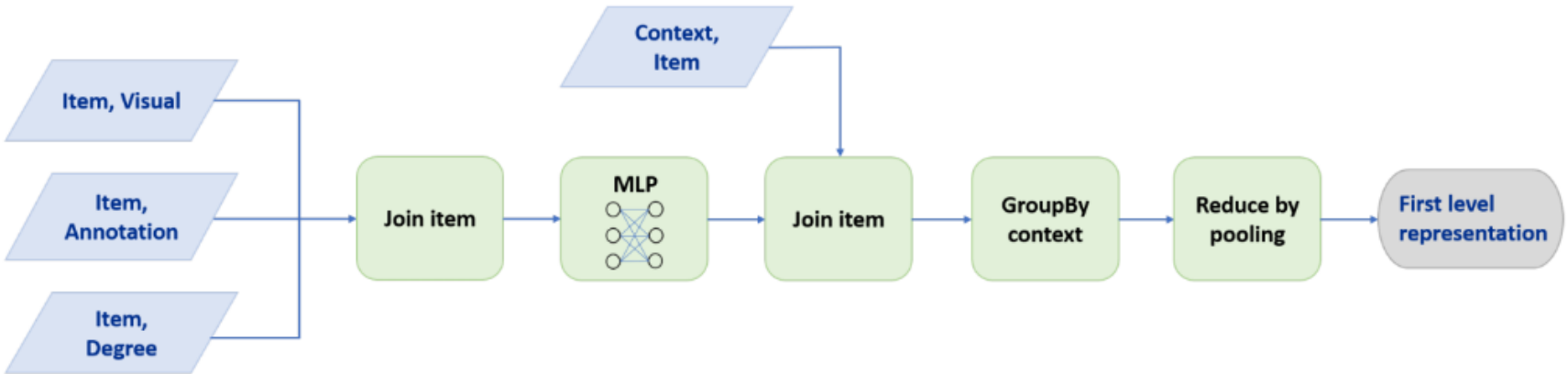
Large Scale RecSys: Training

CPU (producer):

- Select a batch of pins
- Run random walks (for PPR approximation)
- Construct their computation graphs

GPU (consumer):

- Multi-layer aggregations
- Loss computation
- Backprop



from Leskovec et al., 2018

Large Scale RecSys: Training

- Include more and more hard negative samples for each epoch

$$\mathcal{L} = \sum_{(u,v)\in\mathcal{D}} \max(0, -\mathbf{z}_u^\top \mathbf{z}_v + \mathbf{z}_u^\top \mathbf{z}_n + \Delta)$$

- $\mathcal{D}$: set of training pairs from user logs
- $\mathbf{z}_u^\top \mathbf{z}_v$: "positive"/true training pair
- $\mathbf{z}_n$: "negative" sample
- Δ: "margin" (i.e., how much larger positive pair similarity should be compared to negative)

Source pin

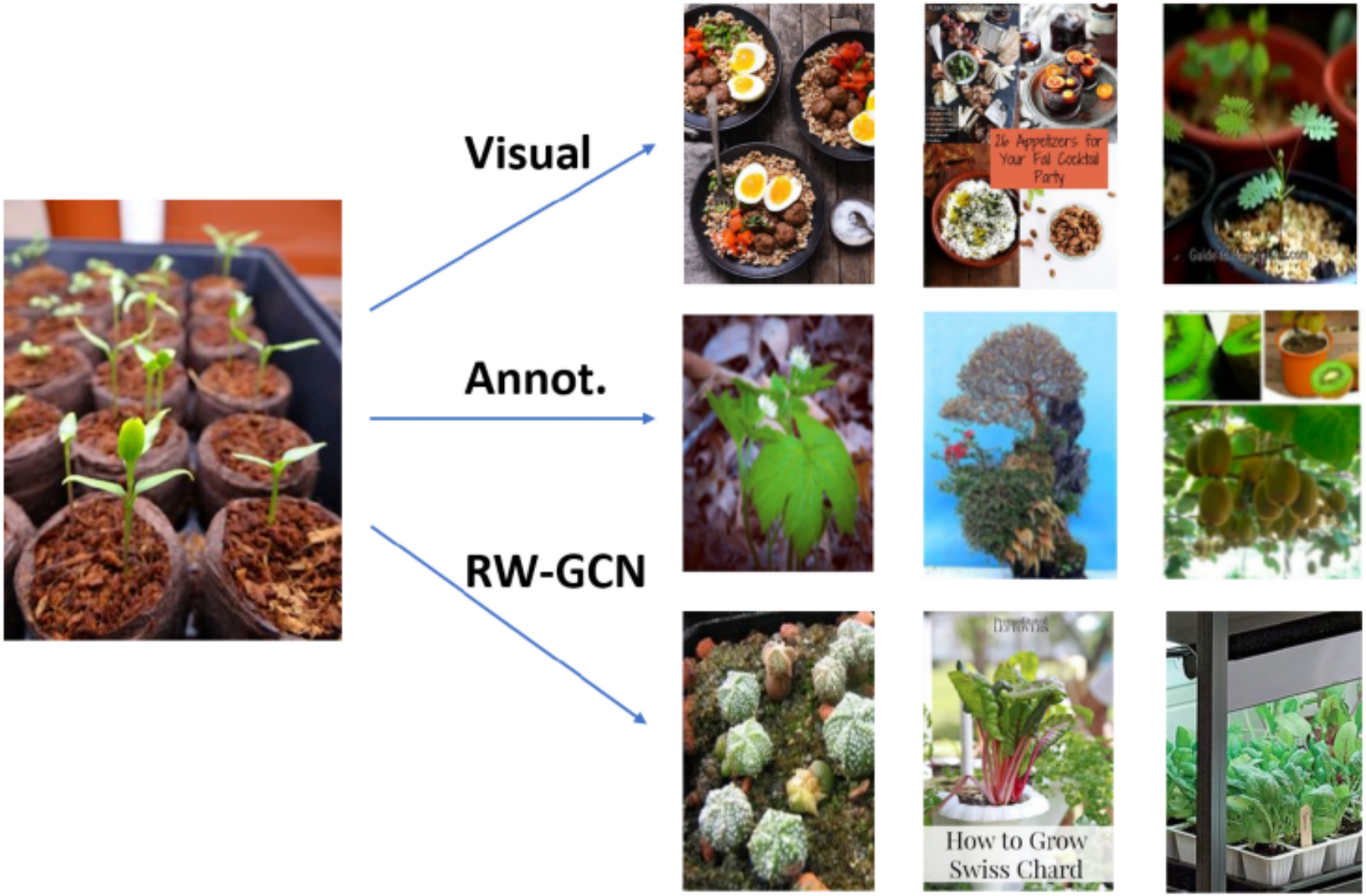
Positive

Easy negative

Hard negative

from Leskovec et al., 2018

Large Scale RecSys: Visual Comparison



Open Problems

Open Problems: Edge embedding

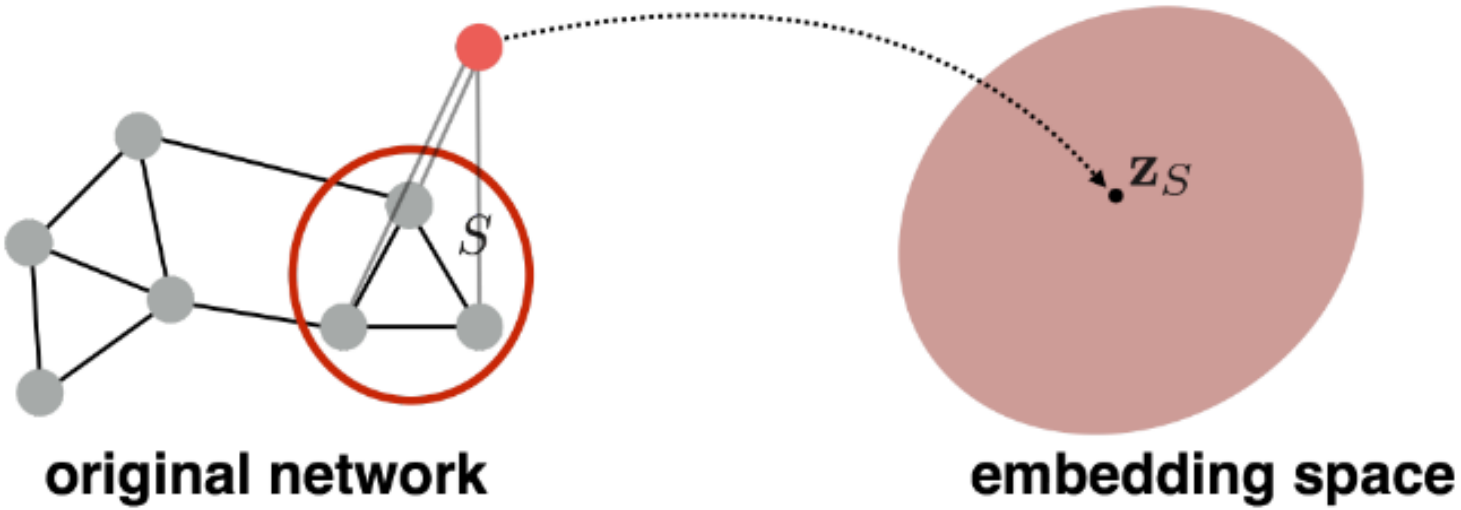
- What is the best way to compose edge feature?

Symmetry operator	Definition
Average	$\frac{f_i(u) + f_i(v)}{2}$
Hadamard	$f_i(u) \cdot f_i(v)$
Weighted-L_1	$\lvert f_i(u) - f_i(v) \rvert$
Weighted-L_2	$(f_i(u) - f_i(v))^2$
Neighbor Weighted-L_1	$\left\lvert \frac{\sum_{w \in N(u) \cup \{u\}} f_i(w)}{\lvert N(u) \rvert + 1} - \frac{\sum_{t \in N(v) \cup \{v\}} f_i(t)}{\lvert N(v) \rvert + 1} \right\rvert$
Neighbor Weighted-L_2	$\left(\frac{\sum_{w \in N(u) \cup \{u\}} f_i(w)}{\lvert N(u) \rvert + 1} - \frac{\sum_{t \in N(v) \cup \{v\}} f_i(t)}{\lvert N(v) \rvert + 1} \right)^2$

from Makarov et al., 2019

Open Problems: Subgraph embedding

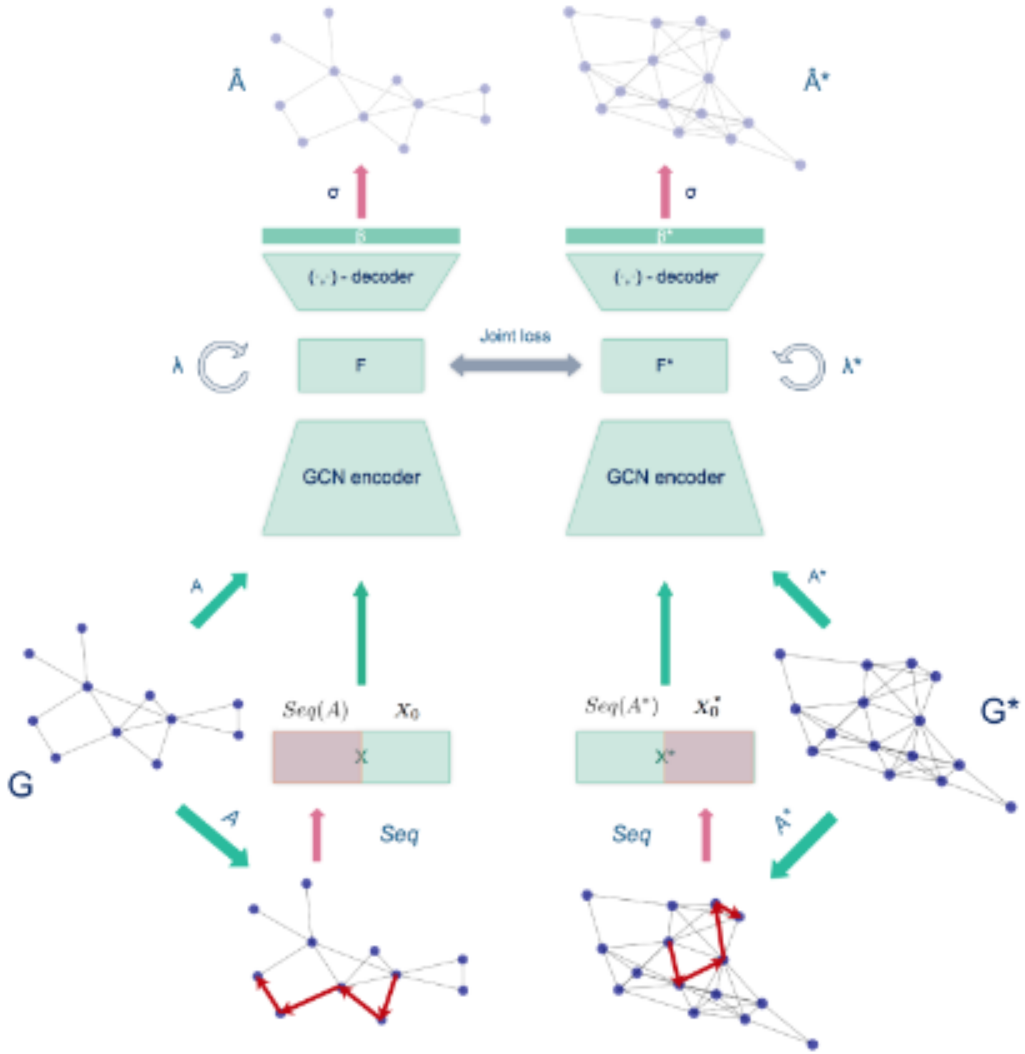
- Even for triangle it is an open question.
- Use sum of embeddings
- Use virtual supernode (same as for whole graph embedding)



from Leskovec et al., 2018

Open Problems: Node & Edge embedding

- How to optimize joint node and edge features?



Open Problems: Text + Graph Fusion

- How to fuse partially-correlated text embeddings and graph embeddings?

Figure 1. TF-IDF, Sent2Vec and DeepWalk embeddings visualization on Cora

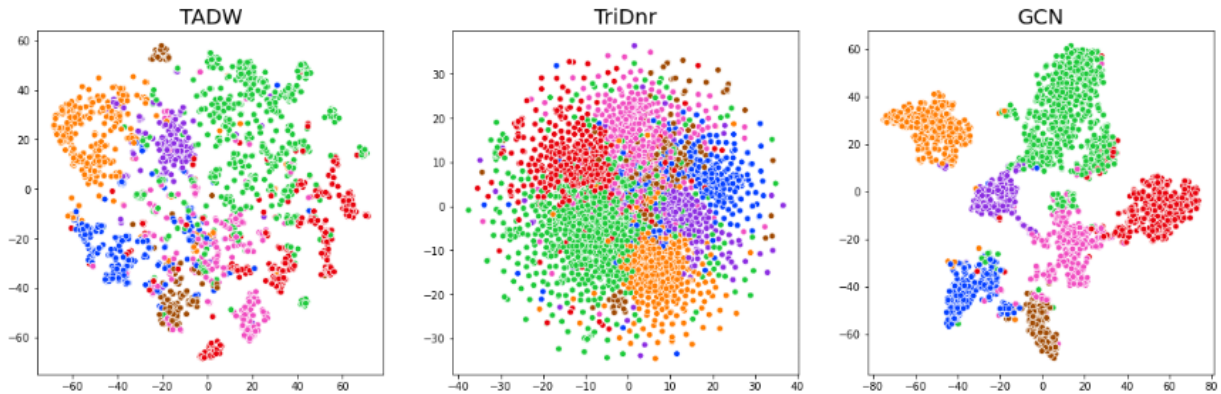
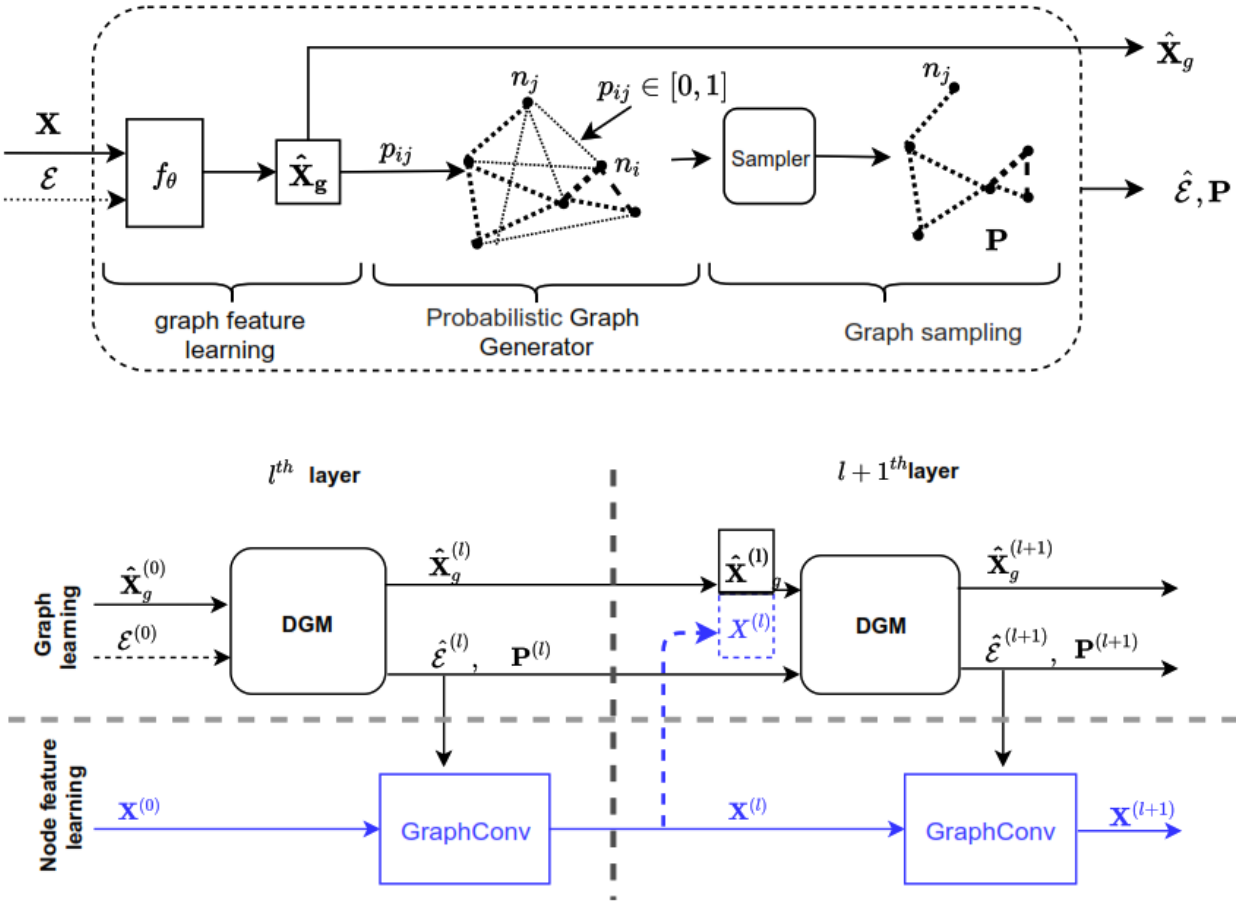


Figure 2. TADW, TriDnr and GCN embeddings visualization on Cora

from Makarov et al., 2021

Open Problems: Graphs from Metric Learning

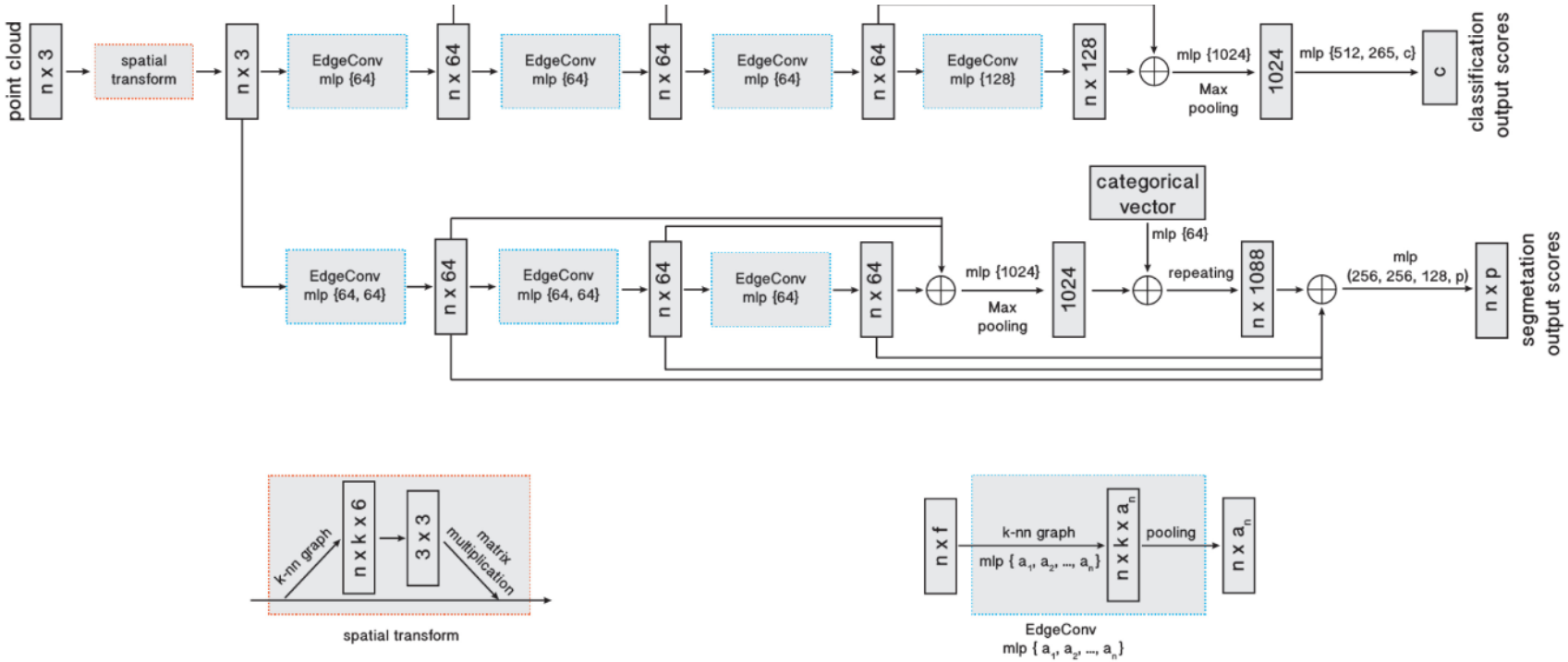
- How to work with non-stationary graph obtained from geometric learning?



Differentiable Graph Module (DGM) for Graph Convolutional Networks from Bronshtein et al., 2020

Open Problems: Graphs from Metric Learning

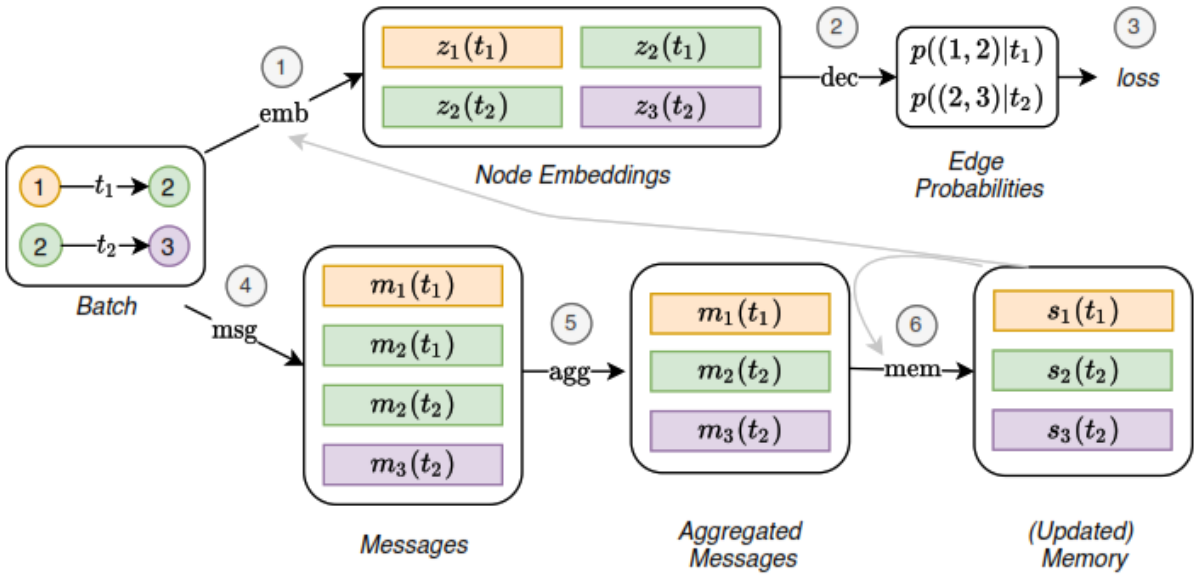
- How to work with non-stationary graph obtained from geometric learning?



Dynamic Graph CNN for Learning on Point Clouds from Solomon et al., 2019

Open Problems: Temporal Graphs

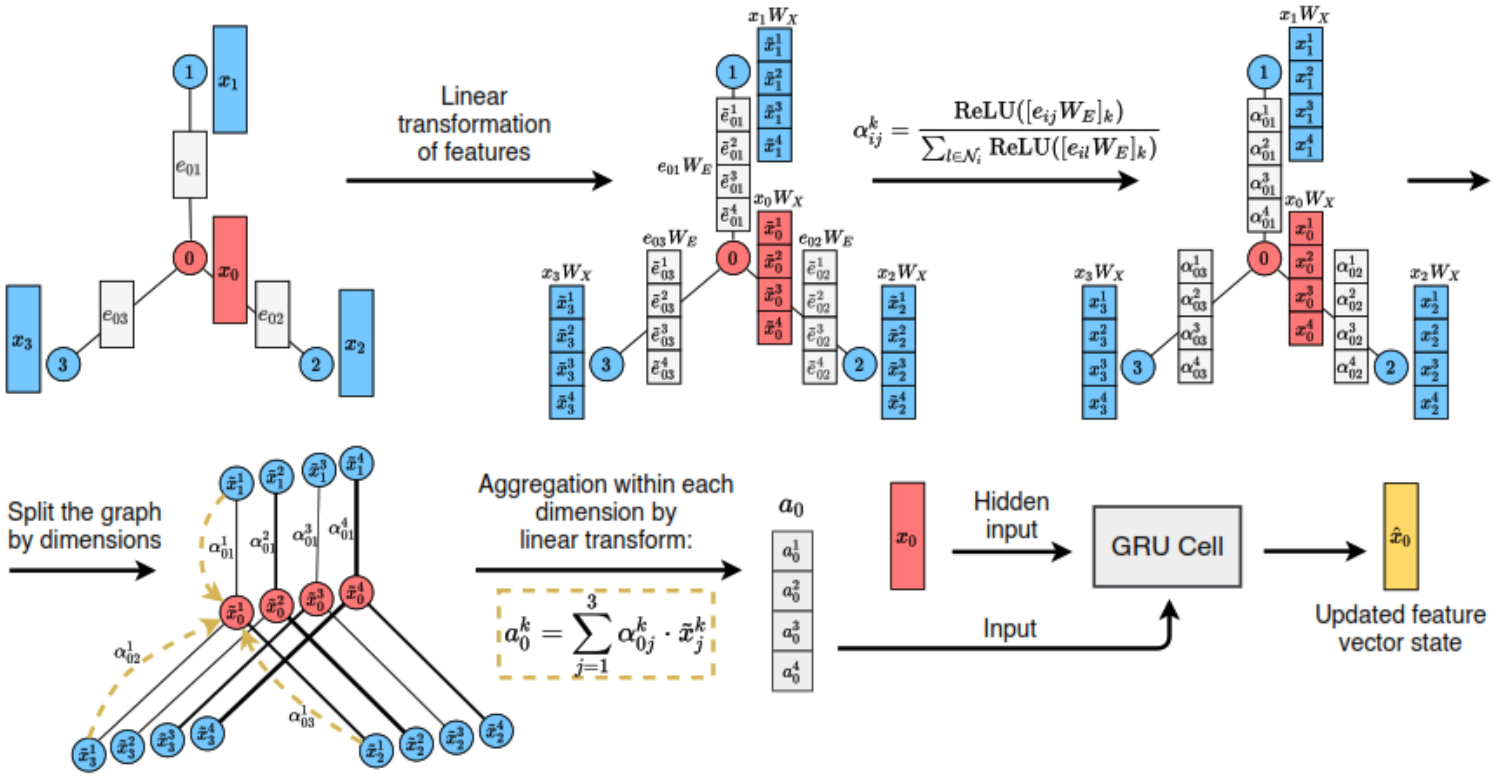
- How to work with large dynamic networks?



TEMPORAL GRAPH NETWORKS FOR DEEP LEARNING ON DYNAMIC GRAPHS from Bronshtein et al., 2019

Open Problems: Temporal Graphs

- How to work with large dynamic networks?



EWS-GCN by Sberbank, 2020

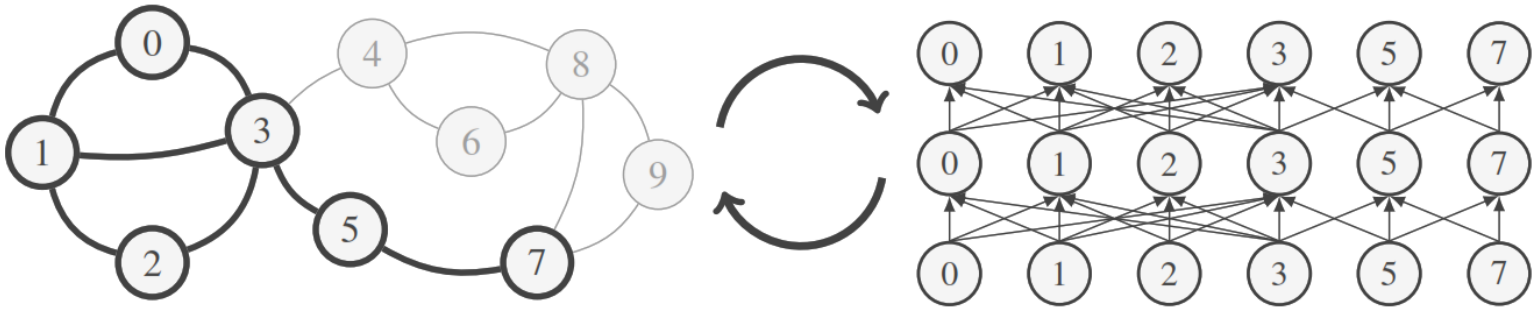
Open Problems: What else?

- How to choose embedding?
- How to mix embeddings and pretrain/initialize?
- How to fuse (heterogeneous) graphs and futures?
- How to speed-up GCN and other models?
- Graph RecSys still struggle from cold start problem!
- Transfer learning and GNN AutoML is hard to improve!
- Working with large dynamic graphs with changing features is still hard!

State-of-the-art

GraphSaint

- Sample from graph and train FC GCN



$\mathcal{G}_s = \texttt{SAMPLE}(\mathcal{G})$ Full GCN on $\mathcal{G}_s$

Algorithm 1 `GraphSAINT` training algorithm

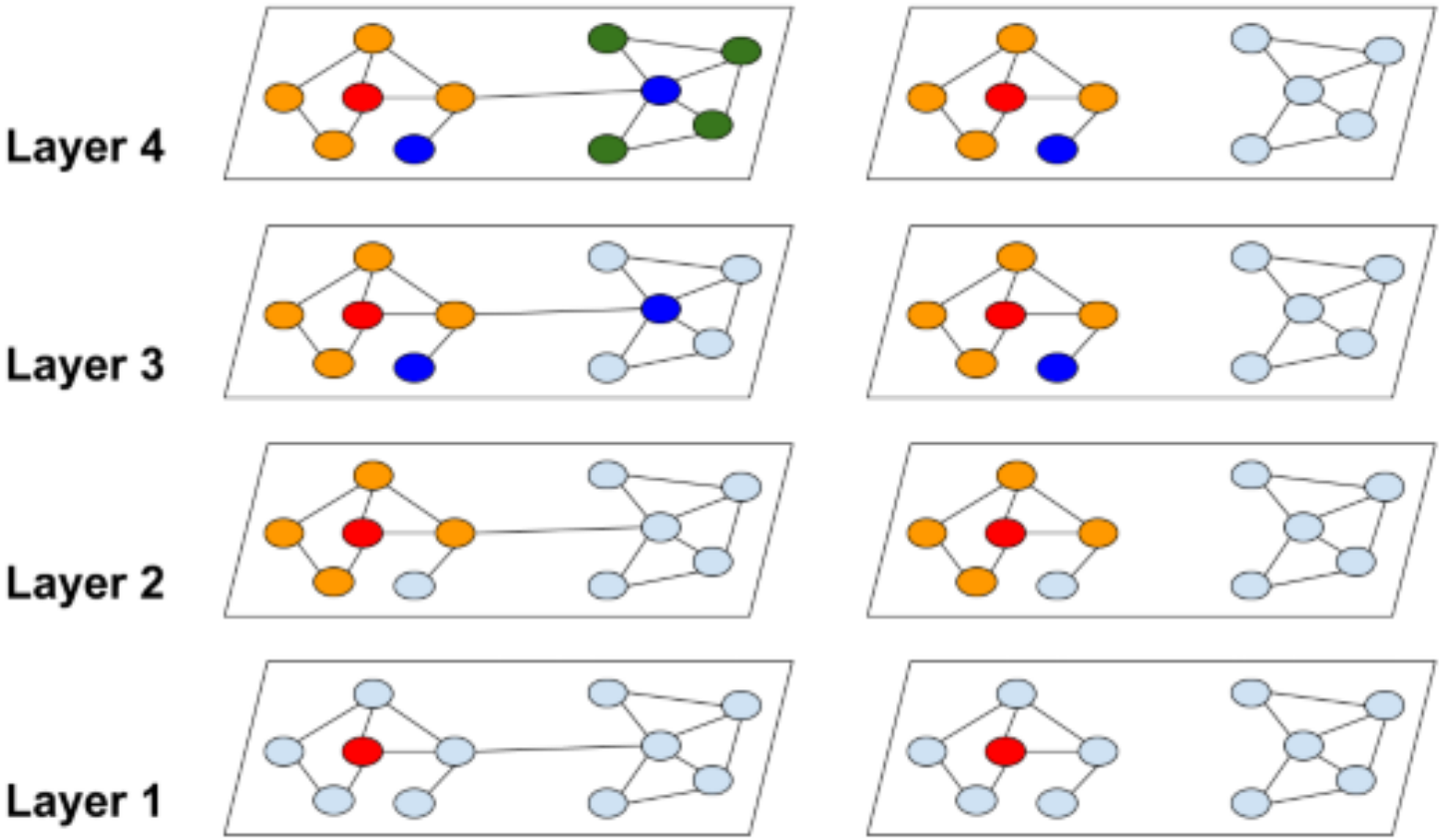
Input: Training graph $\mathcal{G}(\mathcal{V}, \mathcal{E}, \boldsymbol{X})$; Labels $\overline{\boldsymbol{Y}}$; Sampler `SAMPLE`;
Output: GCN model with trained weights

1: Pre-processing: Setup `SAMPLE` parameters; Compute normalization coefficients α, λ.
2: **for** each minibatch **do**
3: $\quad \mathcal{G}_s(\mathcal{V}_s, \mathcal{E}_s) \leftarrow$ Sampled sub-graph of $\mathcal{G}$ according to `SAMPLE`
4: $\quad$ GCN construction on $\mathcal{G}_s$.
5: $\quad \{\boldsymbol{y}_v \mid v \in \mathcal{V}_s\} \leftarrow$ Forward propagation of $\{\boldsymbol{x}_v \mid v \in \mathcal{V}_s\}$, normalized by α
6: $\quad$ Backward propagation from λ-normalized loss $L(\boldsymbol{y}_v, \overline{\boldsymbol{y}}_v)$. Update weights.
7: **end for**

University of Southern California, 2019

ClusterGCN

- Limit Sampling by Cluster properties via RWs

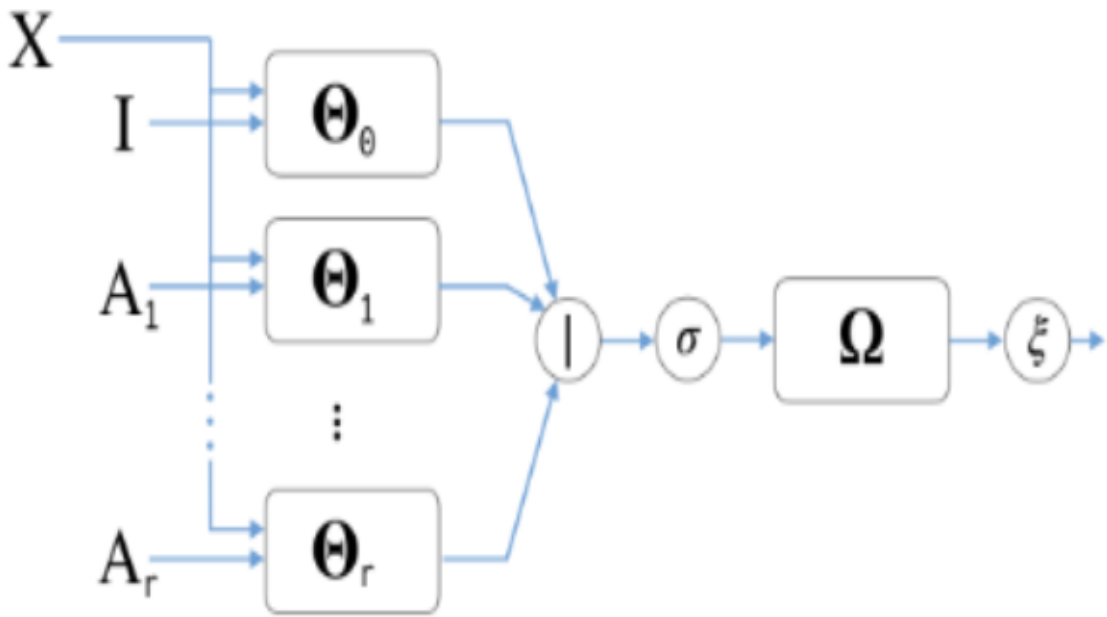


Google Research, University of California, 2020

SIGN

- Precompute diffusion-based sampling instead of stacking more layers

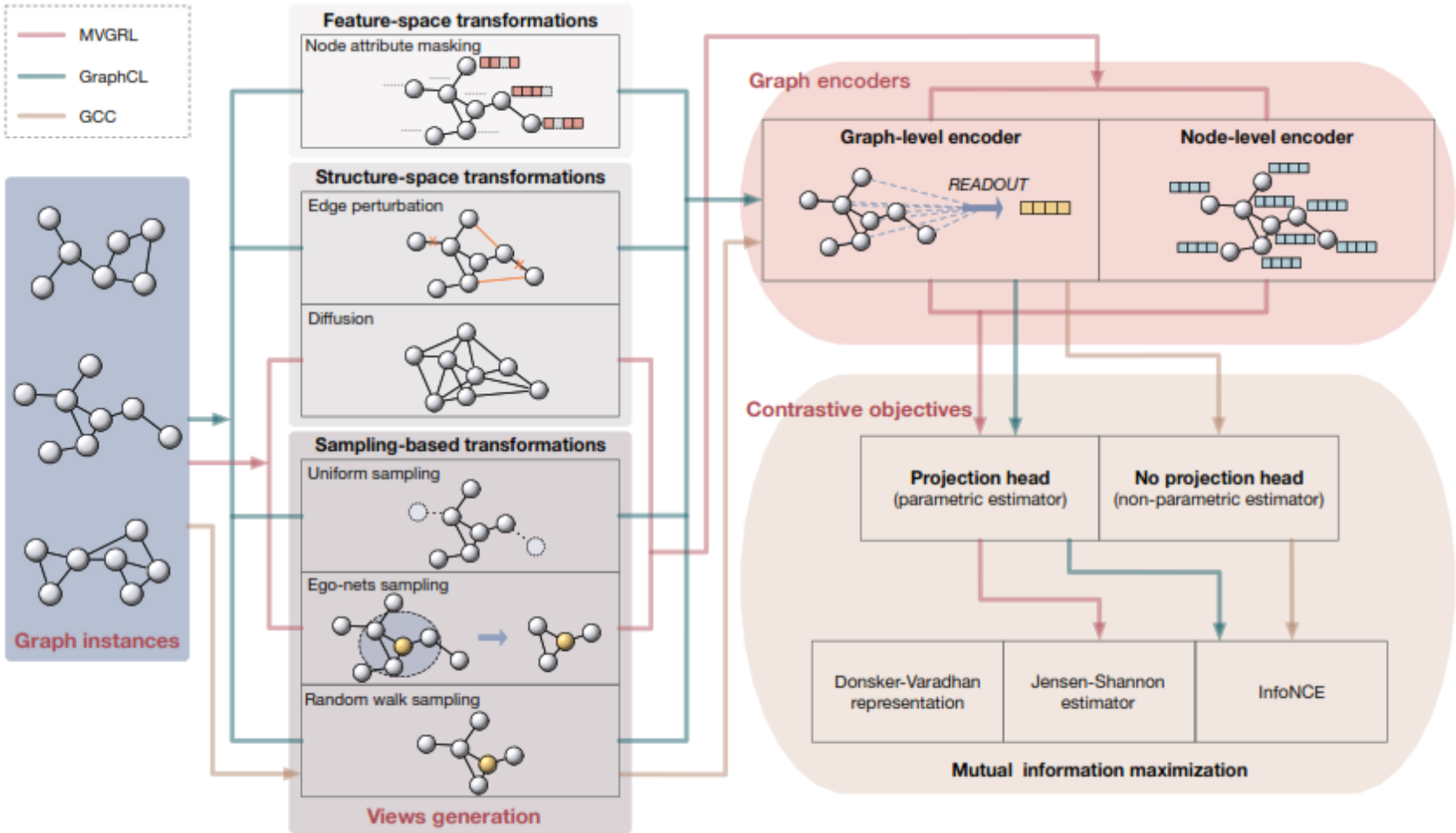
$$\mathbf{Y} = \xi(\tilde{\mathbf{A}}^L \mathbf{X} \mathbf{\Theta}^{(1)} \dots \mathbf{\Theta}^{(L)}) = \xi(\tilde{\mathbf{A}}^L \mathbf{X} \mathbf{\Theta}).$$



Twitter, Imperial College London, 2020

Self-supervised GML

- Contrastive learning / graph augmentation



Amazon, Texas A&M University, 2021

Applications

- ML: NAS & AutoML
- NLP: context embeddings, BERT as transformer solves LP
- CV: 3D point clouds, few-shot learning, KG for captioning
- DM: KG extraction, mining relations
- RecSys: Embedding of everything, tensor decomposition
- RL: Model MDP states via GCN embeddings
- Biology/Chemistry: drug discovery, protein interaction, new materials

Libraries:

- DGL, pyG, DGM, etc.
- "awesome graph embedding"

References (GNNs)

- Scarselli, Franco, Sweah Liang Yong, Marco Gori, Markus Hagenbuchner, Ah Chung Tsoi, and Marco Maggini. "Graph neural networks for ranking web pages." In The 2005 IC on Web Intelligence (WI'05), pp. 666-672. IEEE, 2005.
- Kipf, Thomas N., and Max Welling. "Semi-supervised classification with graph convolutional networks." arXiv preprint arXiv:1609.02907. 2016.
- Veličković, Petar, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. "Graph attention networks." arXiv preprint arXiv:1710.10903. 2017.
- Ying, Rex, Ruining He, Kaifeng Chen, Pong Eksombatchai, William L. Hamilton, and Jure Leskovec. "Graph convolutional neural networks for web-scale recommender systems." In Proceedings of the 24th ACM SIGKDD, pp. 974-983. 2018.

References (Modern GNNs)

- Zeng, Hanqing, Hongkuan Zhou, Ajitesh Srivastava, Rajgopal Kannan, and Viktor Prasanna. "Graphsaint: Graph sampling based inductive learning method." arXiv preprint arXiv:1907.04931. 2019.
- Chiang, Wei-Lin, Xuanqing Liu, Si Si, Yang Li, Samy Bengio, and Cho-Jui Hsieh. "Cluster-GCN: An efficient algorithm for training deep and large graph convolutional networks." In Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp. 257-266. 2019.
- Rossi, Emanuele, Fabrizio Frasca, Ben Chamberlain, Davide Eynard, Michael Bronstein, and Federico Monti. "SIGN: Scalable Inception Graph Neural Networks." arXiv preprint arXiv:2004.11198. 2020.

References (structural)

- B. Perozzi, R. Al-Rfou, and S. Skiena. "Deepwalk: Online learning of social representations." In Proceedings of the 20th ACM SIGKDD international conference , pp. 701-710. 2014.
- J. Tang, M. Qu, M. Wang, M. Zhang, J. Yan, and Q. Mei. "Line: Large-scale information network embedding." In Proceedings of the 24th WWW international conference , pp. 1067-1077. 2015.
- A. Grover and J. Leskovec. "node2vec: Scalable feature learning for networks." In Proceedings of the 22nd ACM SIGKDD international conference, pp. 855-864. 2016.
- S. Abu-El-Haija, B. Perozzi, and R. Al-Rfou. "Learning edge representations via low-rank asymmetric projections." In Proceedings of the 2017 ACM CIKM conference, pp. 1787-1796. 2017.
- H. Cai, V.W. Zheng, and K.C.C. Chang. "A comprehensive survey of graph embedding: Problems, techniques, and applications." IEEE Transactions on Knowledge and Data Engineering 30, no. 9: 1616-1637, 2018