Intelligent Agents
GNNs, ExpressGNN, pLogicNet, MLN Learning

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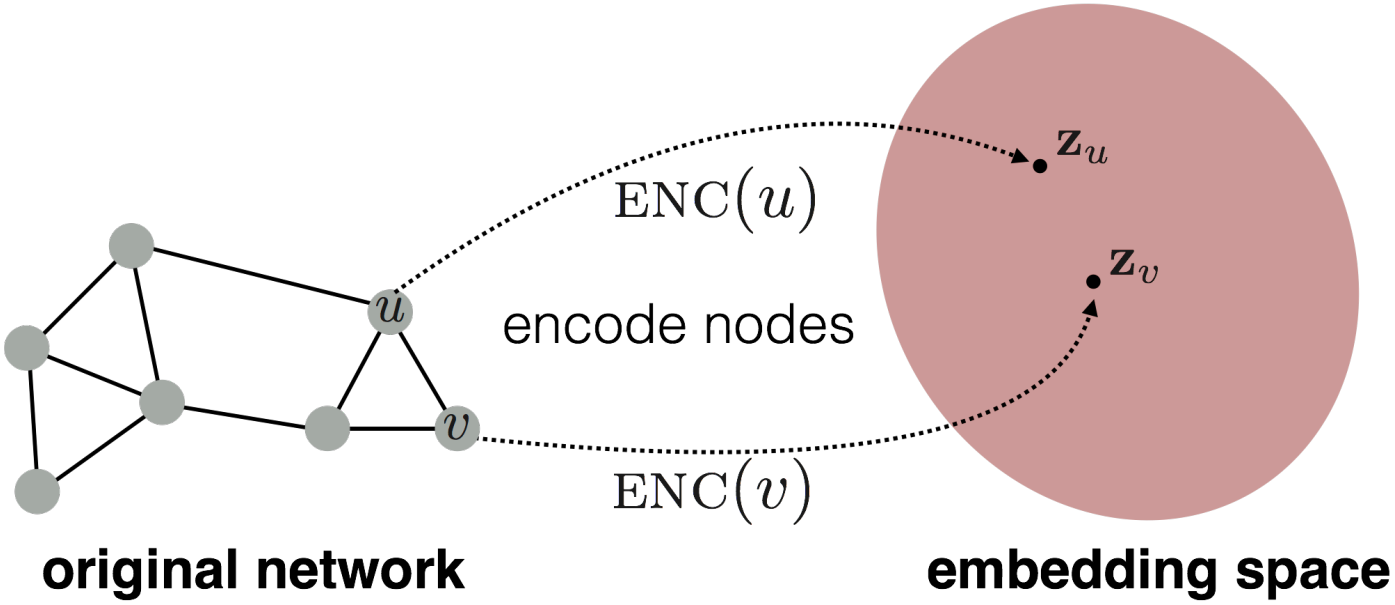
Acknowledgements

- Slides for this presentation are taken from
  - Representation Learning on Networks
    snap.stanford.edu/proj/embeddings-www, WWW 2018
  - Efficient Probabilistic Logic Reasoning with Graph Neural Networks
    Yuyu Zhang, Xinshi Chen, Yuan Yang, Arun Ramamurthy, Bo Li, Yuan Qi & Le Song (slides taken from a presentation by Hengda Shi, Gaohong Liu and Jian Weng)
  - Probabilistic Logic Neural Network for Reasoning, Meng Qu, Jian Tang (slides taken from a presentation by Zijie Huang, Roshni Iyer, Alex Wang)

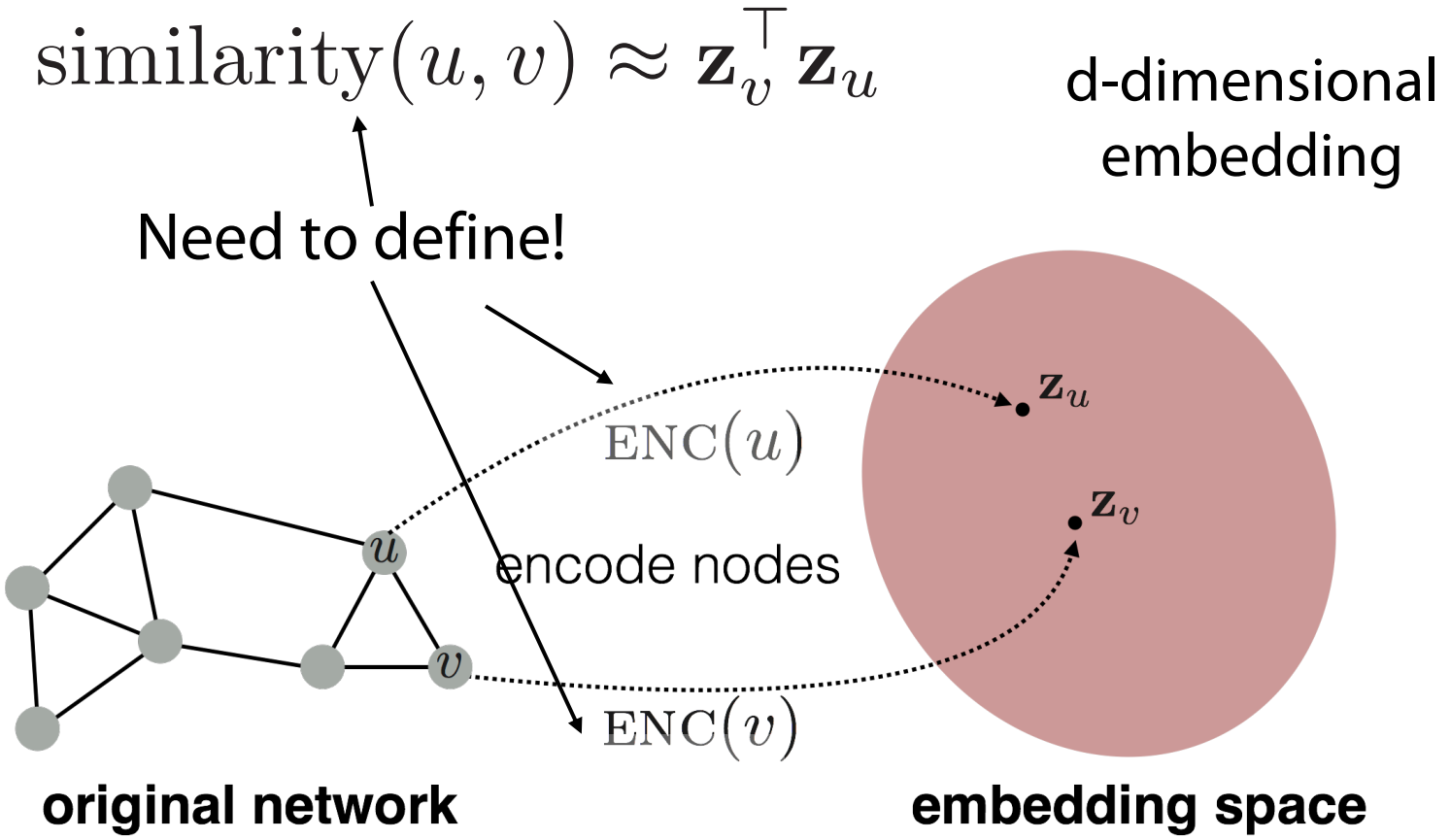
- Slides have been adapted (all faults are mine)

Embedding Nodes

- Encode nodes so that …
  - similarity in the embedding space approximates …
  - similarity in the original network



Embedding Nodes

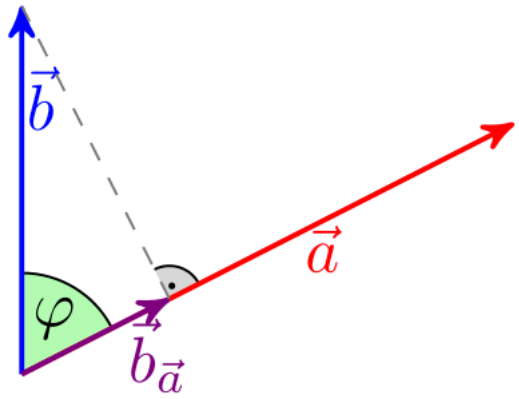


Recap: Dot Product

$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \ \|b_a\|$$

$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \, \|\mathbf{b}\| \cos \ \varphi$$

$$\cos\,(\varphi) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\|\|\mathbf{B}\|} = \frac{\sum_{i=1}^{n} A_i B_i}{\sqrt{\sum_{i=1}^{n} A_i^2} \sqrt{\sum_{i=1}^{n} B_i^2}}$$



Orthogonale Projektion $\vec{b}_{\vec{a}}$ des Vektors $\vec{b}$ auf die durch $\vec{a}$ bestimmte Richtung

Simple ("Shallow") Embedding Approaches

Vectors with d components (with d being a hyperparameter)

Solve optimization problem

- Select embedding vectors for nodes such that "similar" nodes have similar vectors

Various ways to specify similarity of nodes

- Adjacency-based embedding
- Multi-hop embedding
- Random walk approaches

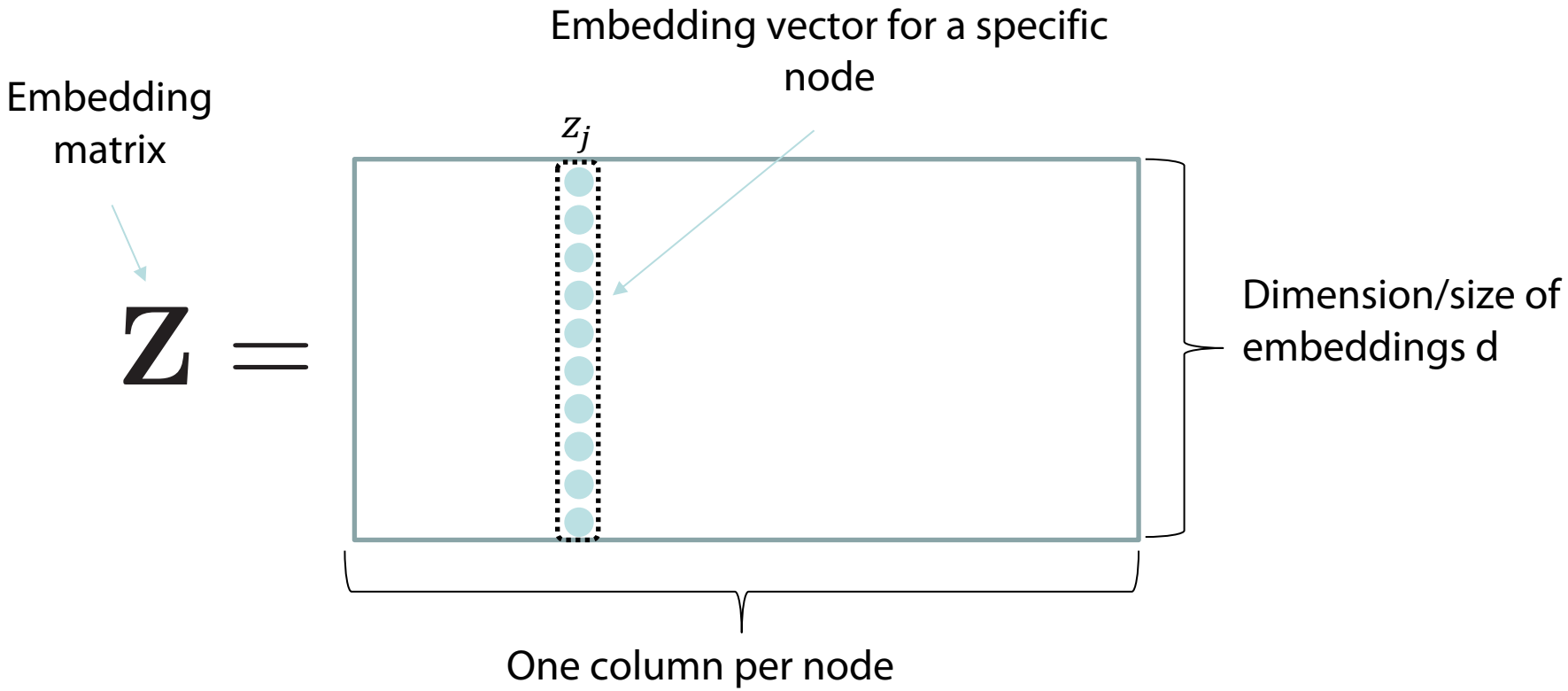
More or less clever approaches, but appropriate similarity features should better be found automatically

$\mathbf{z}_u^\top \mathbf{z}_v \approx$ Probability that *u* and *v* co-occur in a random walk over the network

Hamilton et al. Representation Learning on Graphs: Methods and Applications. IEEE Data Engineering Bulletin on Graph Systems. **2017**.

From “Shallow” to “Deep”

- Shallow: Define features based on selected features



From “Shallow” to “Deep”

- Limitations of shallow encoding:
  - O(|Vd|) parameters needed
    - No parameter sharing
    - Every node has its own unique embedding vector
  - Inherently “transductive” (not inductive)
    - Impossible to generate embeddings for nodes that were not seen during training
  - Does not incorporate node features
    - Many graphs have nodes with features that we can and should leverage

- Need to find embeddings based on holistic view on graph

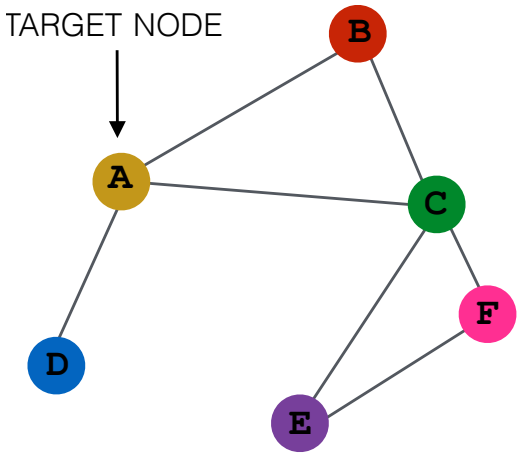
Scarselli et al. The Graph Neural Network Model. IEEE Transactions on Neural Networks. **2005**,

Setup

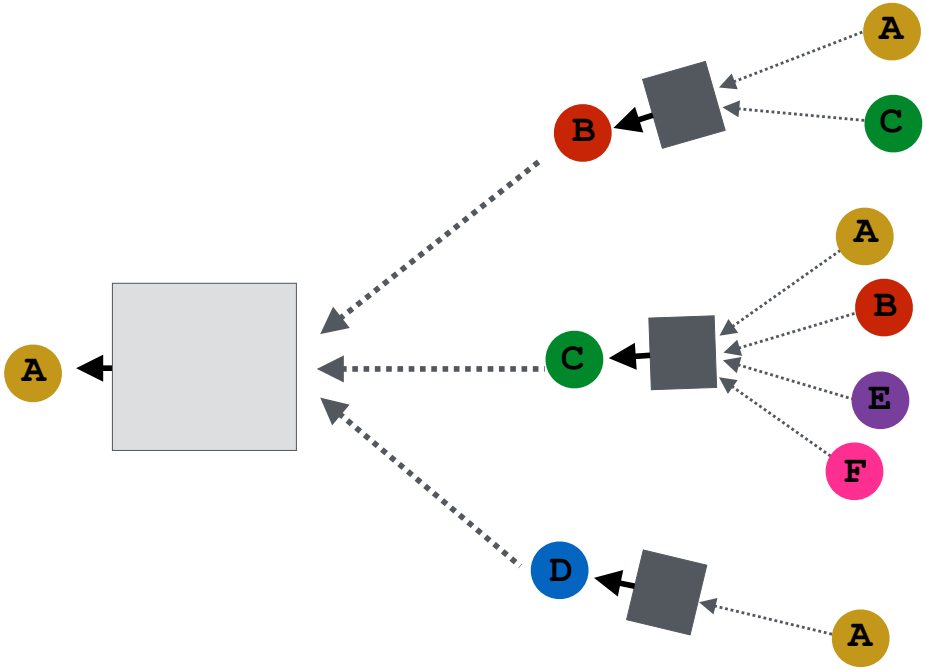
- Assume we have a graph G:
  - V is the vertex set.
  - $\mathbf{A}$ is the adjacency matrix (assume binary).
  - $\mathbf{X} \in \mathbb{R}^{m \times |V|}$ **is a matrix of nodes and their features.**
    - Categorical attributes, text, image data
      - E.g., profile information in a social network.
    - Node degrees, clustering coefficients, etc.
    - Indicator vectors (i.e., one-hot encoding of each node)

Neighborhood Aggregation

- Key idea
  - Generate node embeddings based on local neighborhoods
  - Nodes aggregate information from their neighbor
  - Computation graph for every node

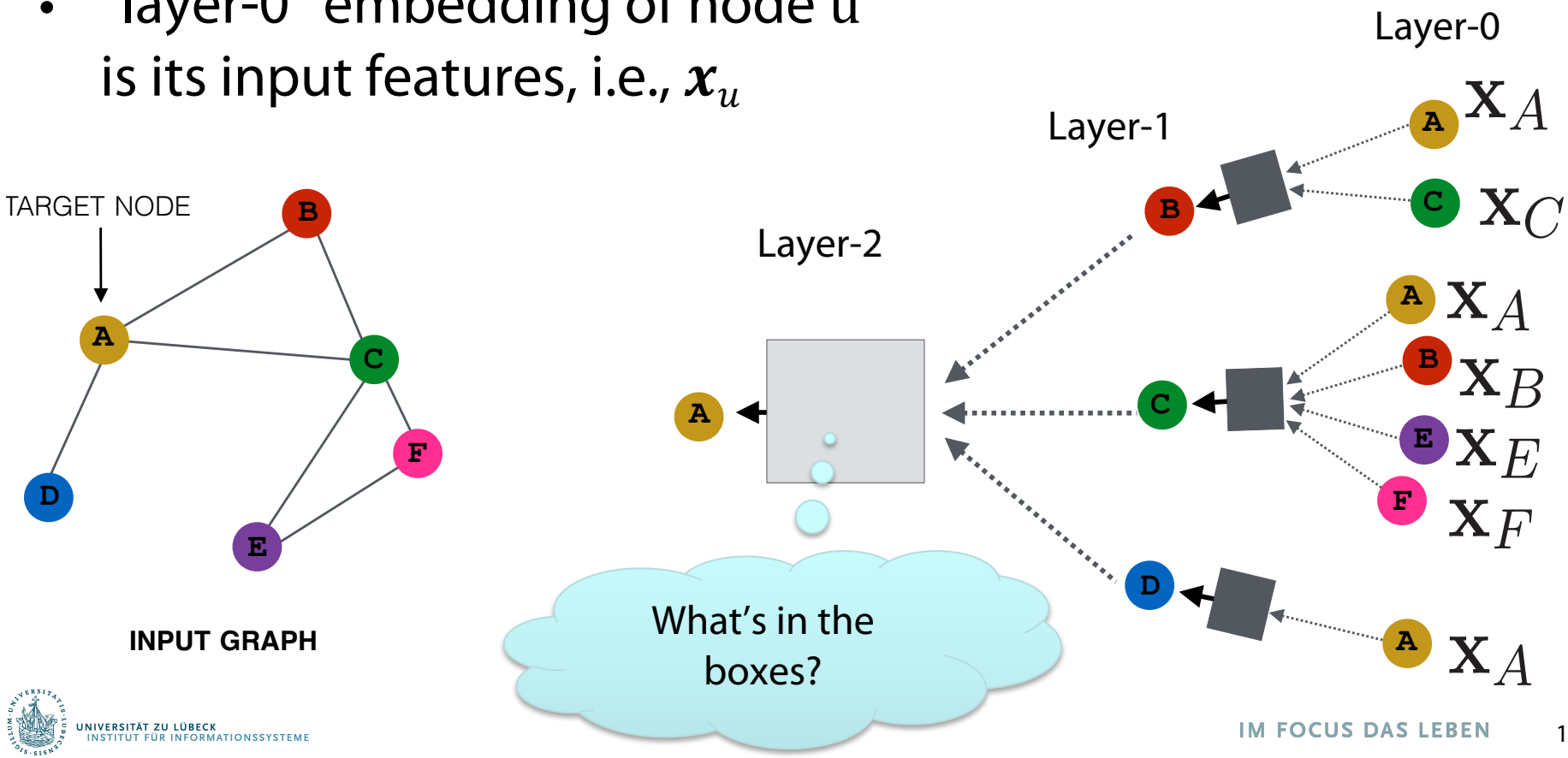


INPUT GRAPH



Neighborhood Aggregation

- Nodes have embeddings at each layer
- Model can be of arbitrary depth
- "layer-0" embedding of node u is its input features, i.e., $\boldsymbol{x}_u$



Graph Networks (GNNs)

- Basic approach: Average neighbor messages and apply a linear transformation with non-linear normalization
- Define a loss function on the embeddings, $\mathcal{L}(z_u)$

Initial "layer 0" embeddings are equal to node features

previous layer embedding of *v*

$$\mathbf{h}_v^0 = \mathbf{x}_v$$

$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right), \quad \forall k > 0$$

kth layer embedding of v

non-linearity (e.g., ReLU or tanh)

average of neighbor's previous layer embeddings

Unsupervised Training

trainable matrices
(i.e., what we learn)

$$\mathbf{h}_v^0 = \mathbf{x}_v$$

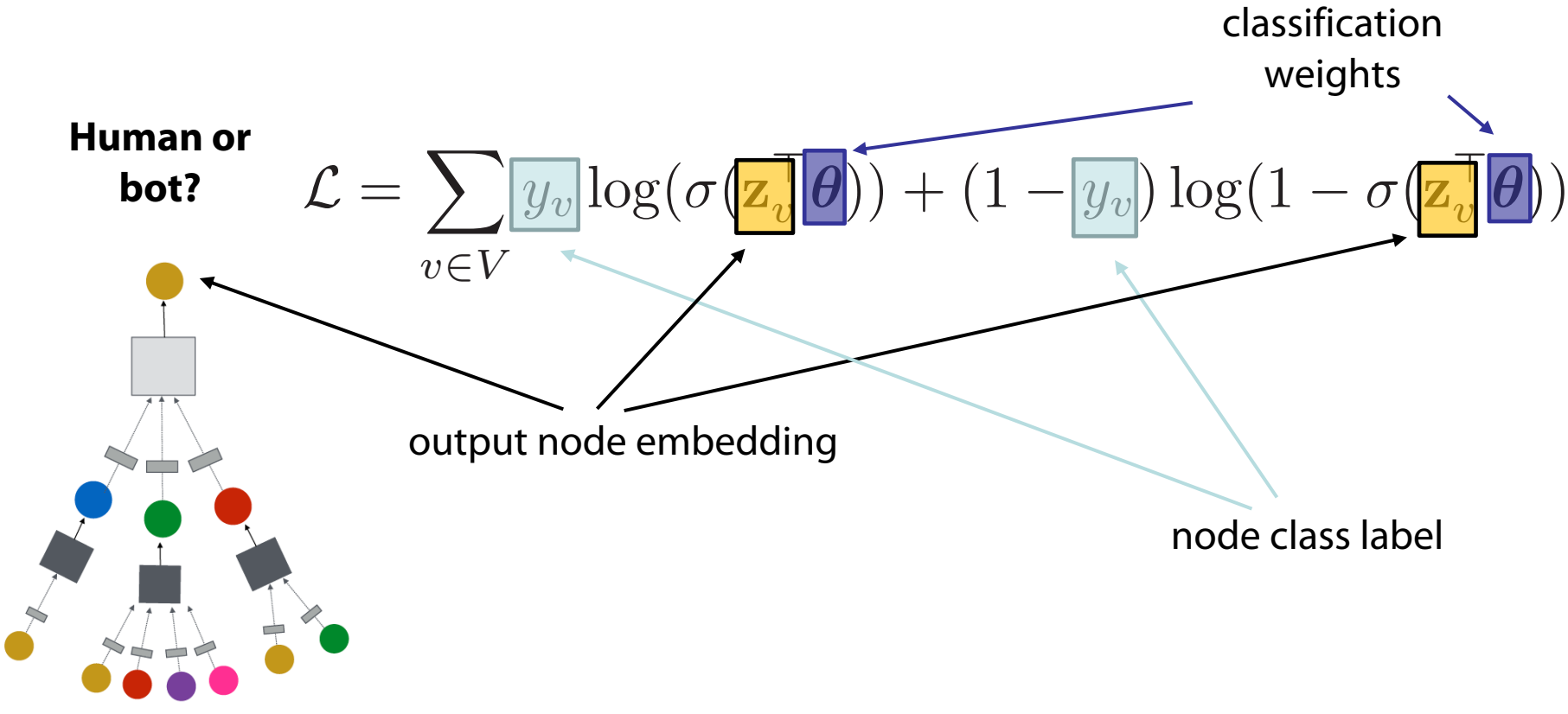
$$\mathbf{h}_v^k = \sigma\left(\mathbf{W}_k \sum_{u \in N(v)} \frac{\mathbf{h}_u^{k-1}}{|N(v)|} + \mathbf{B}_k \mathbf{h}_v^{k-1}\right), \quad \forall k \in \{1, ..., K\}$$

$$\mathbf{z}_v = \mathbf{h}_v^K$$

- After K-layers of neighborhood aggregation, we get output embeddings for each node
- Feed these embeddings into any loss function …
- and run stochastic gradient descent to train the aggregation parameters

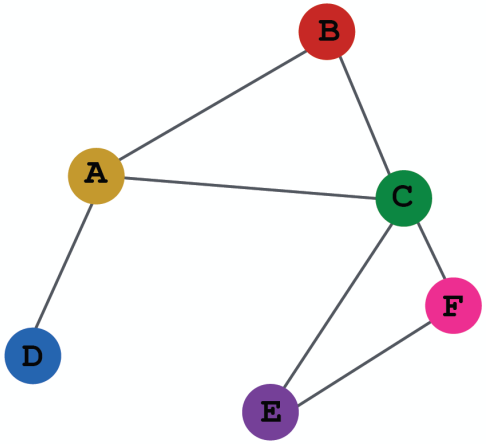
Supervised Training

- E.g., based on node classification $y_v \in \{0, 1\}$:

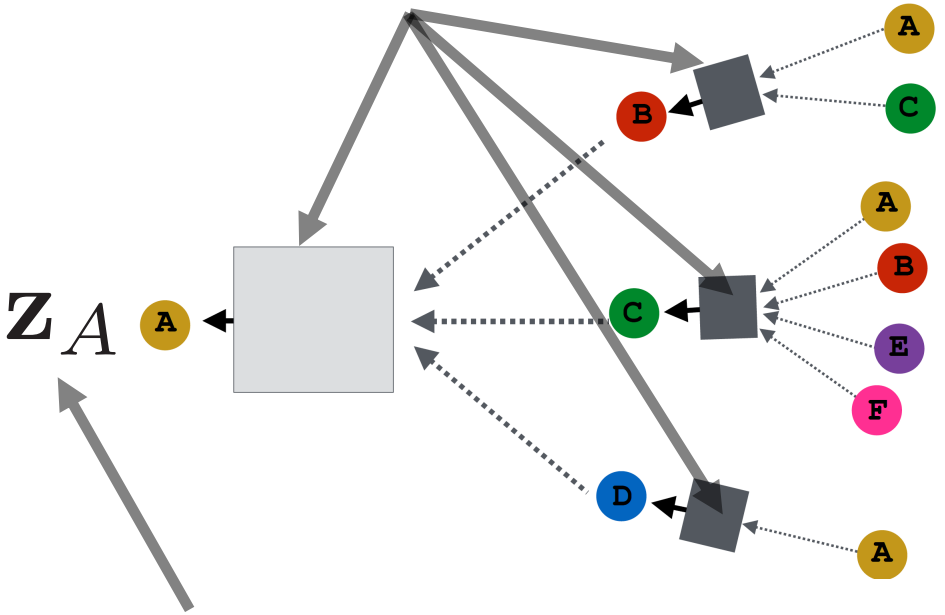


Overview of Model Design

1) Define a neighborhood aggregation function.

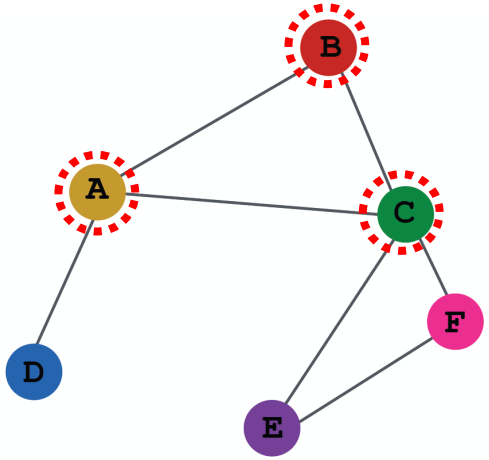


INPUT GRAPH



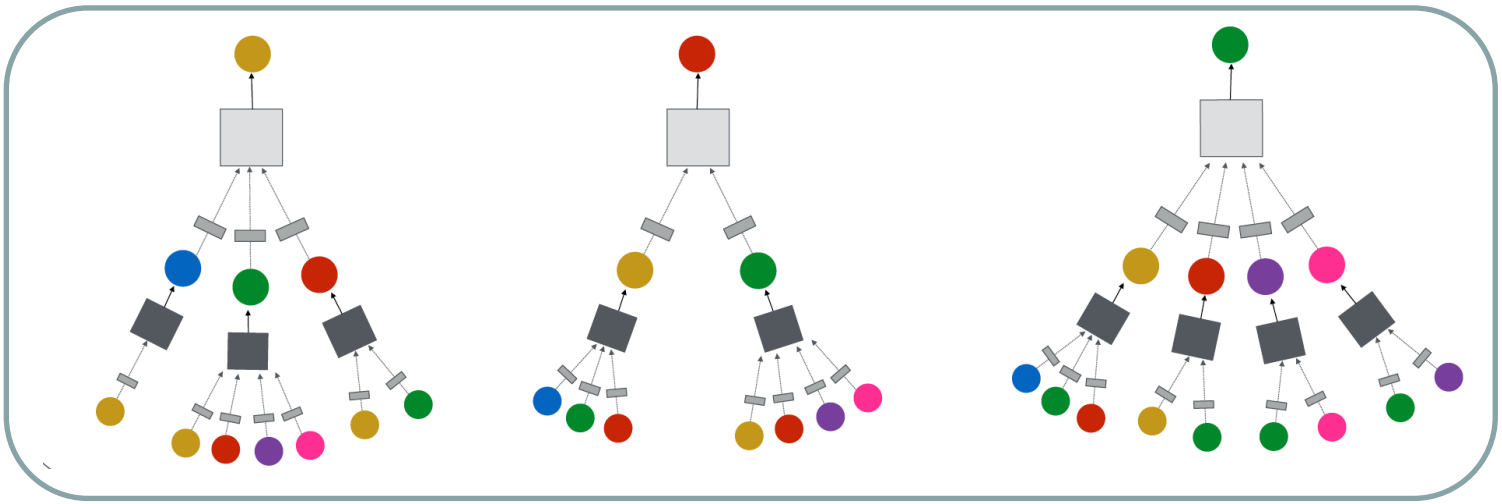
2) Define a loss function on the embeddings, $\mathcal{L}(z_u)$

Overview of Model Design

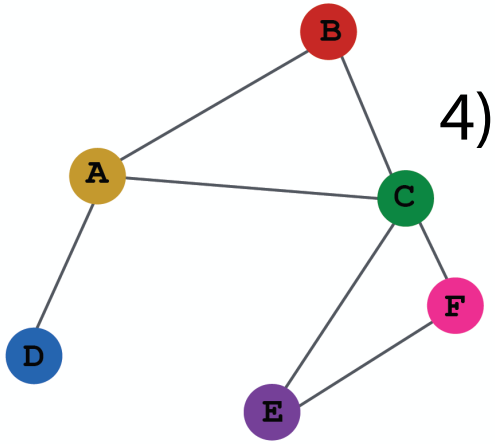


INPUT GRAPH

3) Train on a set of nodes, i.e., a batch of compute graphs



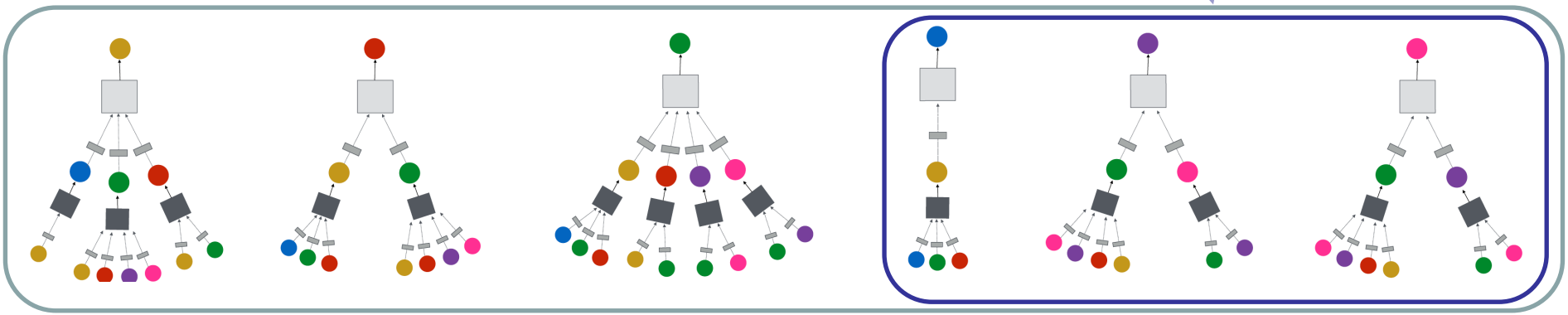
Overview of Model



INPUT GRAPH

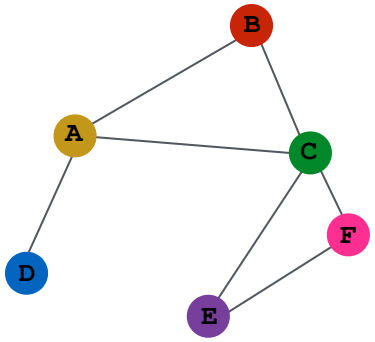
4) Generate embeddings for nodes as needed

Even for nodes we never trained on!!!!

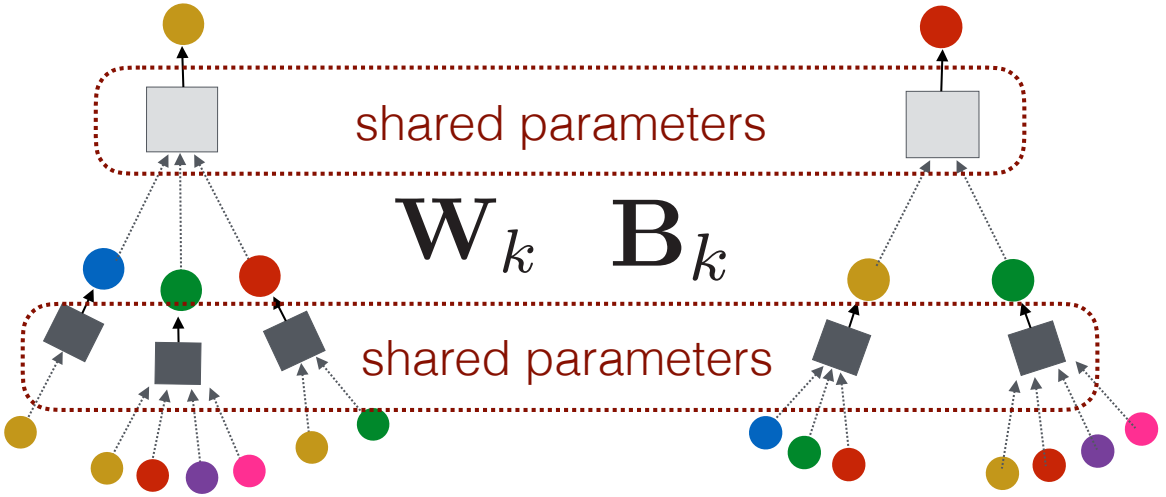


Inductive Capability

- Same aggregation parameters are shared for all nodes.
- Number of model parameters is sublinear in |V| …
- … and we can generalize to unseen nodes!



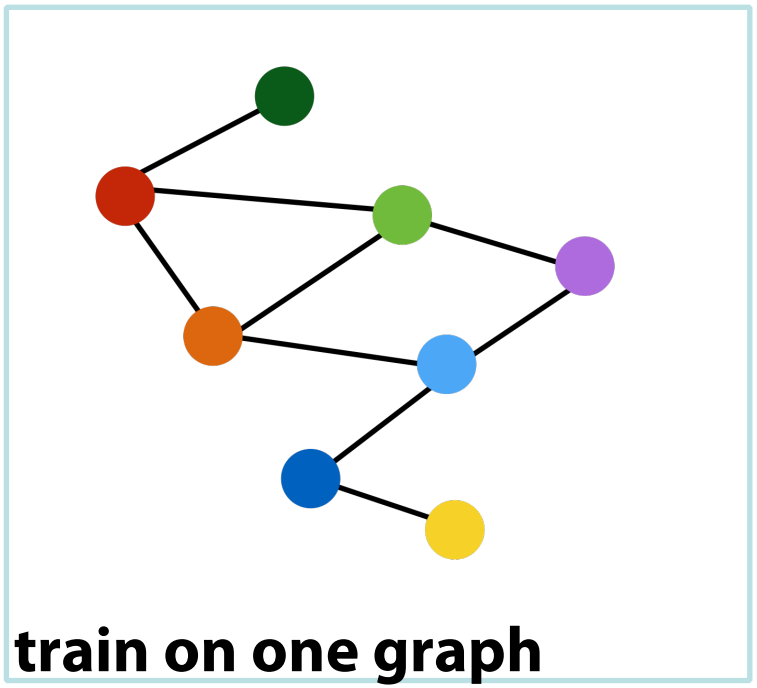
INPUT GRAPH



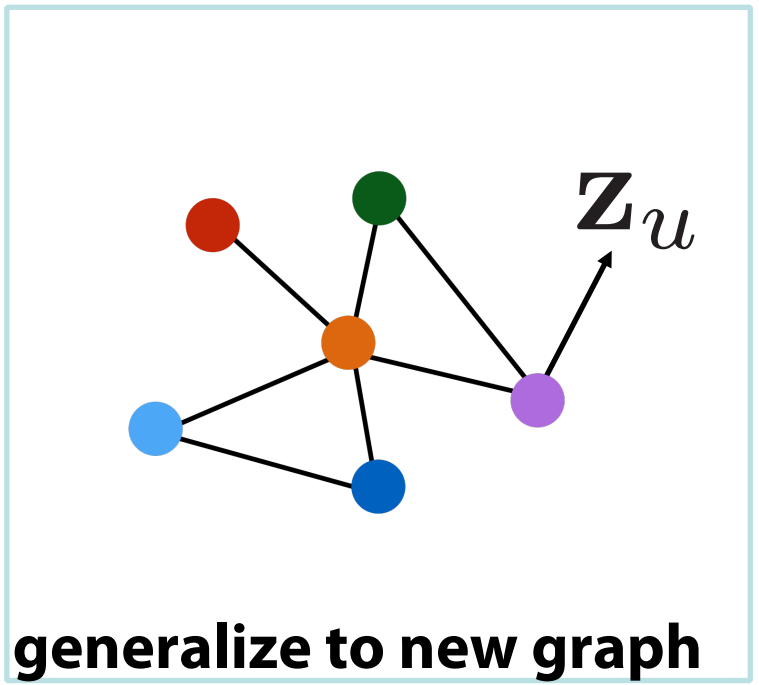
Compute graph for node A

Compute graph for node B

Inductive Capability



train on one graph

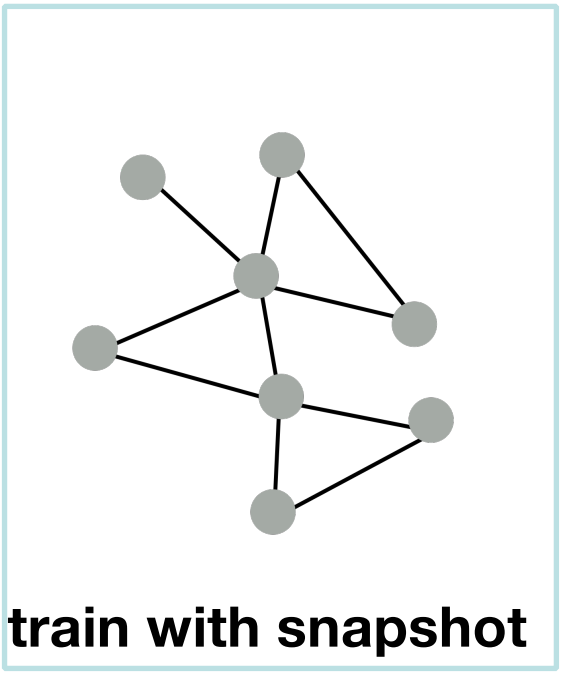


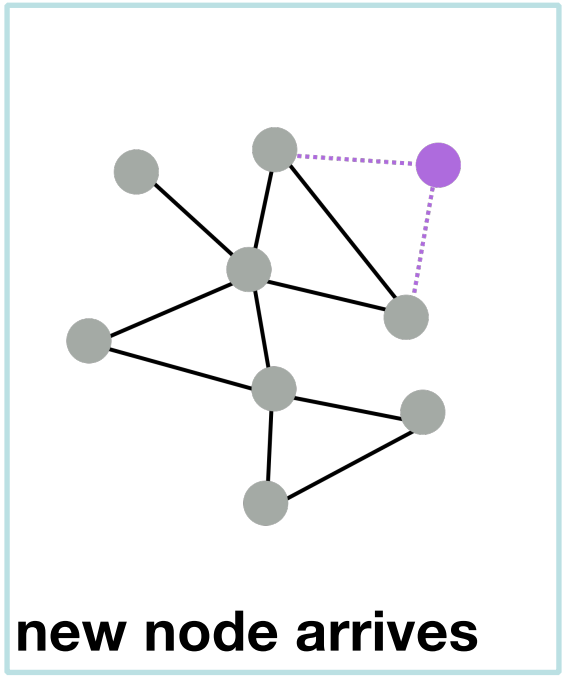
generalize to new graph

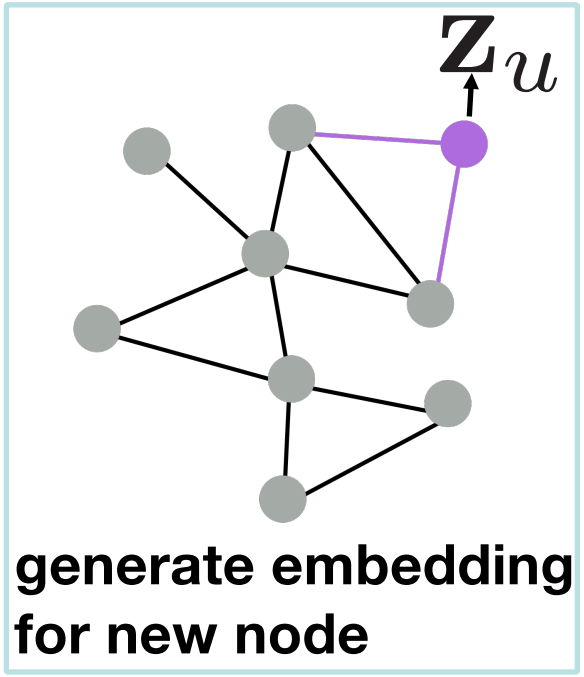
Inductive node embedding → generalize to entirely unseen graphs

e.g., train on protein interaction graph from model organism A and generate embeddings on newly collected data about organism B

Inductive Capability







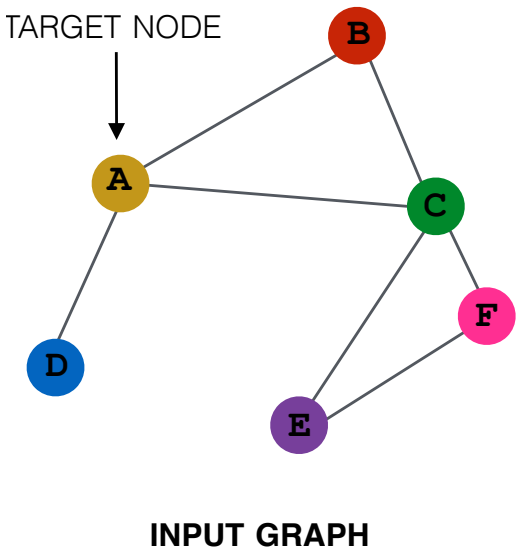
Many application settings constantly encounter previously unseen nodes.

e.g., Reddit, YouTube, GoogleScholar, ….

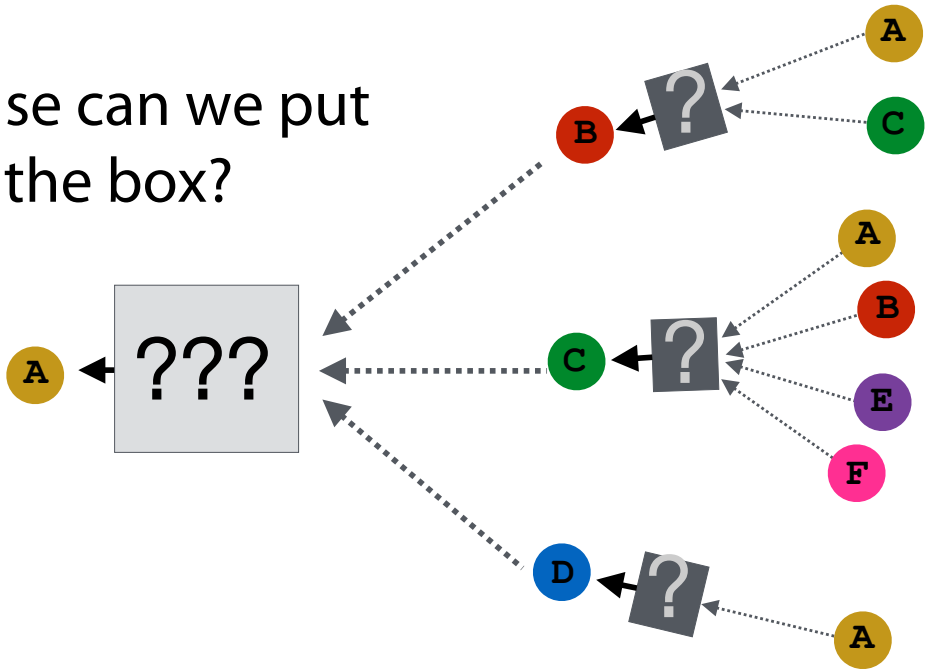
Need to generate new embeddings "on the fly"

Neighborhood Aggregation

- Key distinctions are in how different approaches aggregate messages



What else can we put in the box?



Graph Convolutional Networks (GCNs)

- Slight variation on the neighborhood aggregation idea:

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

same matrix for self and neighbor embeddings

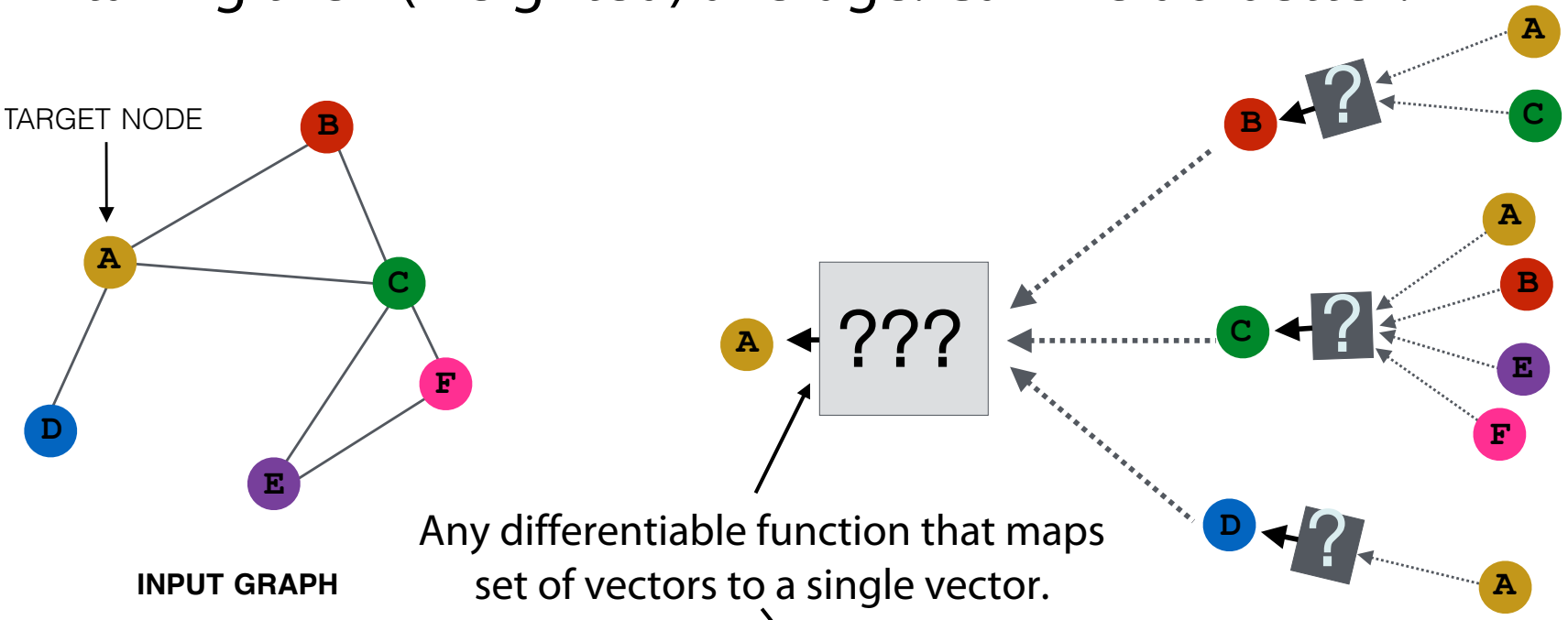
per-neighbor normalization

- Empirically, this configuration to give the best results
  - More parameter sharing
  - Down-weights high degree neighbors

Semi-supervised classification with graph convolutional networks
TN Kipf, M Welling. In Proc. 5th International Conference on Learning Representations (ICLR-17), **2017**.

GraphSAGE (SAmple and aggreGatE)

- So far we have aggregated the neighbor messages by taking their (weighted) average. Can we do better?



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

concatenate self embedding and neighbor embedding

GraphSAGE Variants

- Mean:

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

- Pool:
  - Transform neighbor vectors and apply symmetric vector function

element-wise mean/max

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

- LSTM-based RNNs:
  - Apply LSTM to random permutation of neighbors (LSTMs work on seqences)

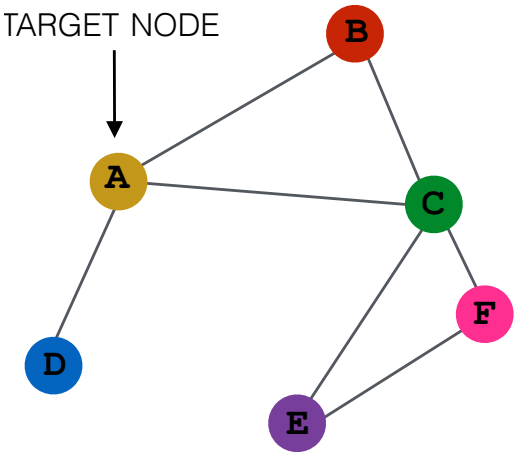
$$\text{AGG} = \text{LSTM}\left([\mathbf{h}_u^{k-1}, \forall u \in \pi(N(v))]\right)$$

- Transformers?

William L. Hamilton, Rex Ying, and Jure Leskovec. 2017. Inductive representation learning on large graphs. In Proc. NIPS'17. **2017**.

Neighborhood Aggregation

- GCNs and GraphSAGE generally only 2-3 layers deep
- What if we want to go deeper?
  - Overfitting from too many parameters.
  - Vanishing/exploding gradients during backpropagation



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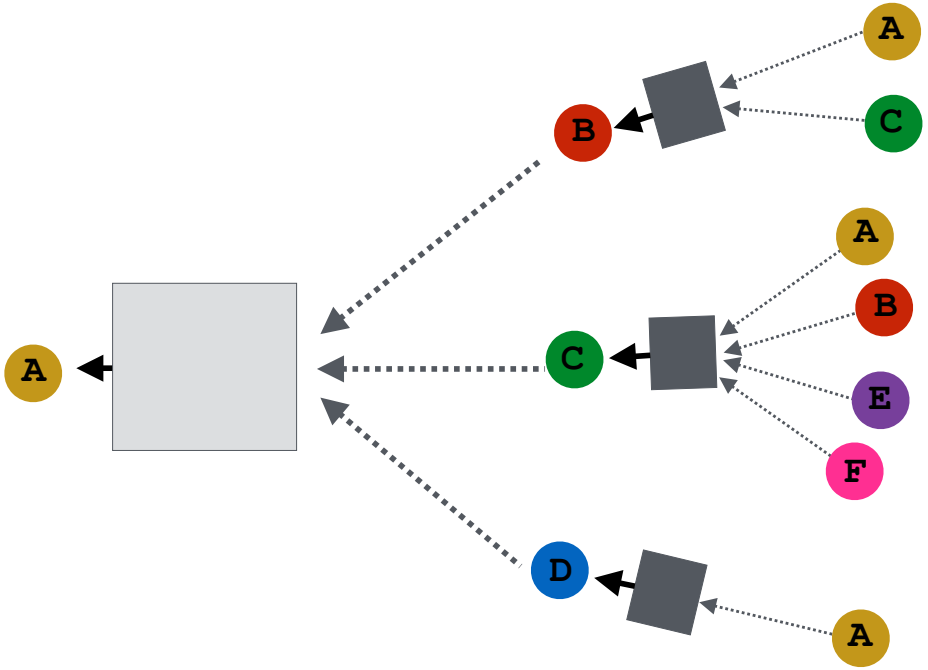
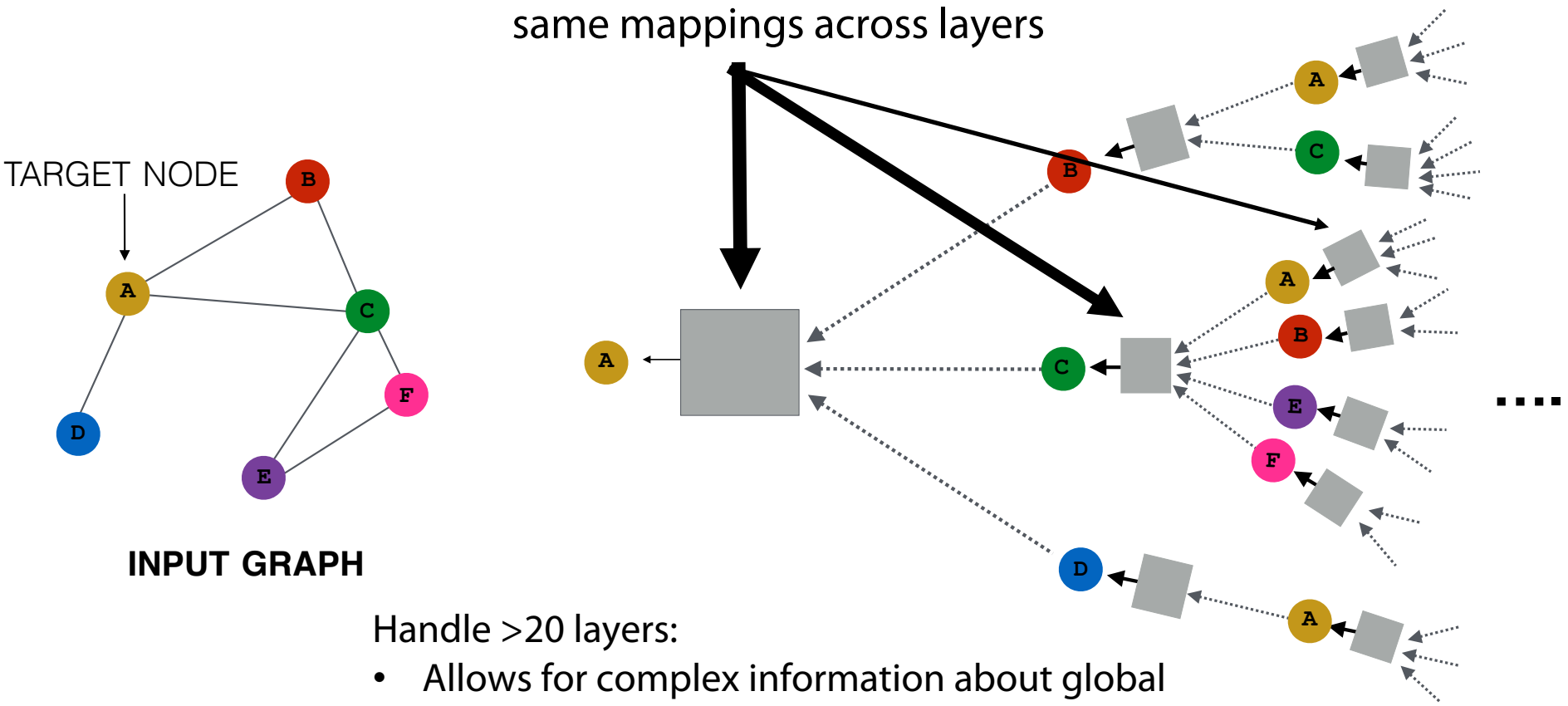


Gated Graph Networks

- Use techniques from recurrent networks
- Parameter sharing across layers, recurrent state update



Handle >20 layers:

- Allows for complex information about global graph structure to be propagated to all nodes

Neighborhood aggregation with RNN state update

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

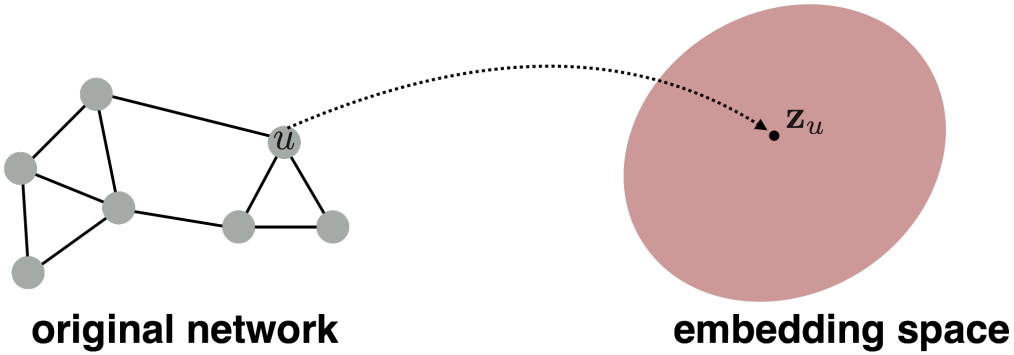
2. Update node "state" using Gated Recurrent Unit (GRU)
   New node state depends on the old state and the message from neighbors:

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

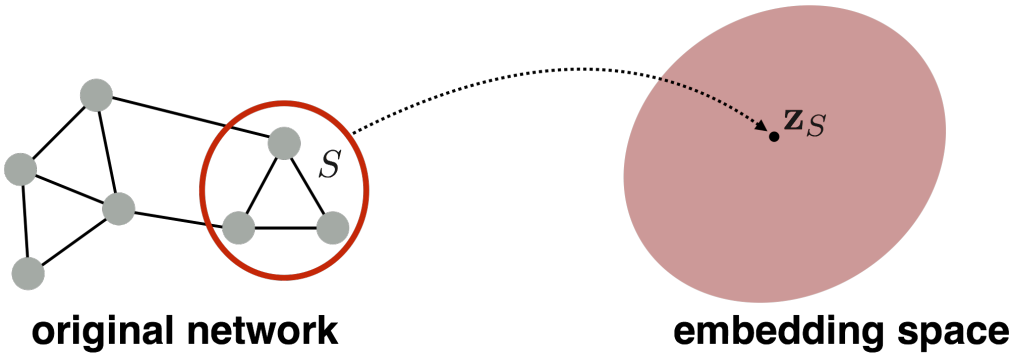
Yujia Li Richard Zemel Marc Brockschmidt Daniel Tarlow,
Gated Graph Sequence Neural Networks
Proceedings of ICLR'16. **2016**.

(Sub)graph Embeddings

- So far we have focused on node-level embeddings…



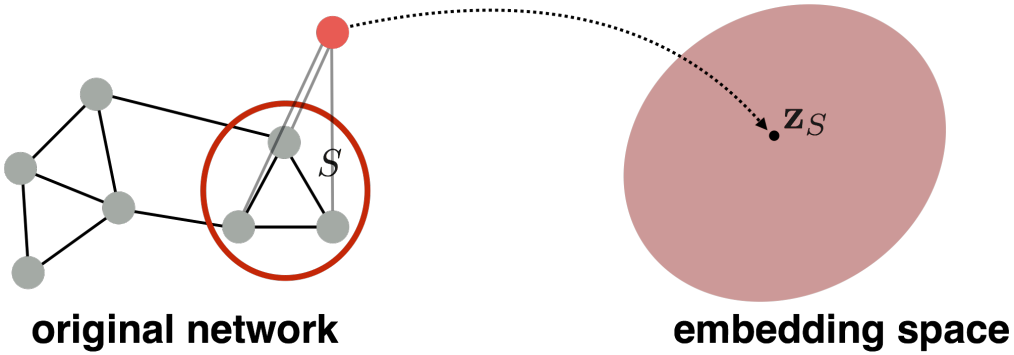
- But what about subgraph embeddings?



(Sub)graph Embeddings

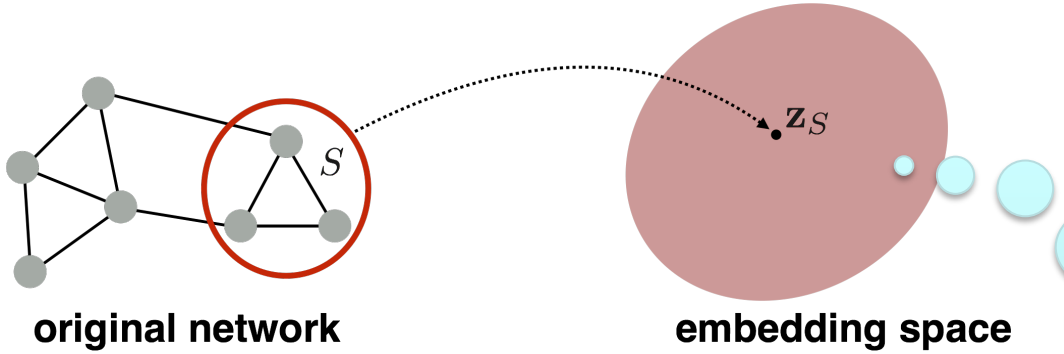
How to embed (sub)graphs with millions or billions of nodes?

- Use representative as a virtual node



Li et al. Gated Graph Sequence Neural Networks. In Proc. ICLR. **2016**.

- Sum or average node embeddings: $\mathbf{z}_S = \sum_{v \in S} \mathbf{z}_v$



How to do the analog of CNN "pooling" on networks?

Duvenaud et al. Convolutional Networks on Graphs for Learning Molecular Fingerprints. In Proc. ICML **2016**.

Summary so far

- Key idea: Generate node embeddings based on local neighborhoods.
  - GraphSAGE
    - Generalized neighborhood aggregation
  - Gated Graph Networks
    - Neighborhood aggregation + recursion (same mappings for a layer) + GRUs
  - Graph Convolutional Networks
    - Average neighborhood information and stack computational networks

Recent Advances in Graph Networks

- Attention-based neighborhood aggregation (Weightings for neighbors)
  - Graph Attention Networks (Velickovic et al., 2018)
  - GeniePath (apaptive receptive paths) (Liu et al., 2018)
- Generalizations based on spectral convolutions (eigen-decomposition of graph Laplacian L)
  - Geometric Deep Learning (Bronstein et al., 2017)
  - Mixture Model CNNs (Monti et al., 2017)
- Speed improvements via subsampling
  - FastGCNs (Chen et al., 2018)
  - Stochastic GCNs (Chen et al., 2017)

$L = D - A$ (degree matrix – adjacency matrix)

Graph Networks, Embeddings, and KGs

- Graph networks allow for the computation of embeddings for nodes in a KG
- With embeddings, existence of links between nodes can be estimated (KG completion)
  - See also, e.g., node2vec
- If nodes originate from words …
- … we have another way to embed nodes
  - See also, e.g., word2vec
  - KG completion based on word embeddings

node2vec: Scalable Feature Learning for Networks. A. Grover, J. Leskovec. ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD), **2016**

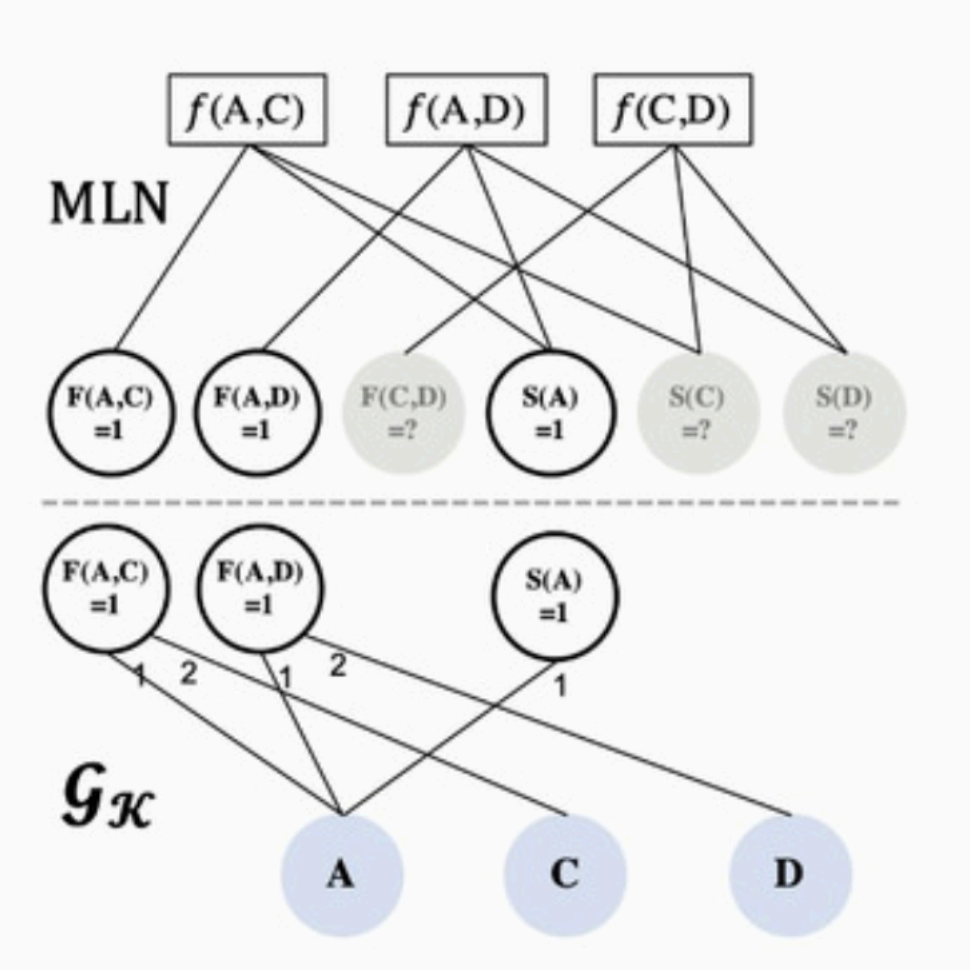
Approaches for Completing KGs

- Graph Network approach
- Embedding approach
- What about probabilistic graphical models?
  - ➢ Markov logic networks for link estimation?

Advantages of MLNs

- Incorporate domain knowledge with first-order logic
  - Composition
    - $\forall X, Y, Z: R_1(X, Y) \wedge R_2(Y, Z) \rightarrow R_3(X, Z)$
  - Inverse relations
    - $\forall X, Y: R_1(X, Y) \rightarrow R_2(Y, X)$
  - Symmetry
    - $\forall X, Y: R_1(X, Y) \rightarrow R_1(Y, X)$
  - Subrelation
    - $\forall X, Y: R_1(X, Y) \rightarrow R_2(X, Y)$

MLNs and Knowledge Graphs



Ground KG of MLN

Knowledge graph
(e.g., from text)
as evidence

Markov Logic Networks

Pros:

- Logic formulas incorporate prior knowledge
- Allows MLN to generalize in tasks with small amount of labeled data

Cons:

- Inference in MLN is computationally intensive
- Logic formulas can only cover a small part of the possible combinations of knowledge graph relations in real-world texts

Graph Networks / Word-based Embeddings

Pros:

- Efficiency – Directly work on KG
- Compactness – GNNs with shared parameters can be memory efficient
- Expressiveness – GNN can capture structure knowledge encoded in the KG, and so-called tunable embeddings can encode entity-specific information (see below)

Cons:

- GNNs do not explicitly incorporate prior knowledge into models and may require many labeled examples for a target task

Combining MLNs and KG Embeddings

- KG Completion
  - With MLN model M_i
  - With embedding approaches
    - GNN-based (ExpressGNN)

      Efficient Probabilistic Logic Reasoning with Graph Neural Networks
      Yuyu Zhang, Xinshi Chen, Yuan Yang, Arun Ramamurthy, Bo Li, Yuan Qi & Le Song.
      In: Proc. ICLR-20. https://iclr.cc/virtual/poster_rJg76kStwH.html **2020**.

    - Embedding based (pLogicNet)

      Probabilistic Logic Neural Network for Reasoning, Meng Qu, Jian Tang.
      In: Proc. NeurIPS-20. https://github.com/DeepGraphLearning/pLogicNet **2019**.

- Learn new MLN model M_{i+1} based on completed KG

Variational EM for MLN Learning

- MLN used to model the joint probabilistic distribution of all observed and latent variables, O and H, respectively

$$P_w(O,H) := \frac{1}{Z(w)} \exp\left(\sum_{f \in F} w_f \sum_{a_f \in A_f} \phi(a_f)\right)$$

- Training an MLN (w, F) means to determine the weights w_f of the formulas $f \in F$
- An MLN can be trained by maximizing the log-likelihood of all observed facts $logP_w(O)$, i.e., $\widehat{w}_{ML} = \underset{w}{argmax} \log P_w(O)$ and $w = \widehat{w}_{ML}$
- Due to intractability caused by hidden variables, instead of optimizing the log-likelihood, we optimize the evidence lower bound (ELBO) s.t.

$$\log P_w(O) \geq L_{ELBO}(Q_\theta, P_w)$$

- The goal is to find a distribution Q_θ that approximates P_w "from below"

E step: Inference

- Infer the posterior distribution of the latent variables, where P_w is fixed and Q_θ is optimized to minimize the KL divergence between $Q_\theta(H|O)$ and $P_w(H|O)$
- Estimate the true posterior with a mean-field approximation
- In mean-field variational approximation, each unobserved ground formula $r(a_r) \in H$ is independently inferred as:

$$Q_\theta(H|O) \coloneqq \prod_{r(a_r)\in H} Q_\theta(r(a_r))$$

- Each $Q_\theta(r(a_r))$ follows a Bernoulli distribution
- Parameterize Q_θ with GNN

a_r is a sequence of parameters that fits the arity of r

$r(a_r) \in H$ is a slight abuse of notation

E step: Inference

- With mean-field approximation, $L_{ELBO}(Q_\theta, P_w)$ can be reorganized as:

$$L_{ELBO}(Q_\theta, P_w) = \mathbb{E}_{Q_\theta(H|O)}[\log P_w(O,H) - \log Q_\theta(H|O)]$$
$$= \mathbb{E}_{Q_\theta(H|O)}\left[\log\left(\frac{1}{Z(w)}\exp\left(\sum_{f\in F} w_f \sum_{a_f \in A_f} \emptyset_f(a_f)\right)\right)\right] - \mathbb{E}_{Q_\theta(H|O)}\left[\log \prod_{r(a_r)\in H} Q_\theta(r(a_r))\right]$$
$$= \mathbb{E}_{Q_\theta(H|O)}\left[\sum_{f\in F} w_f \sum_{a_f \in A_f} \emptyset_f(a_f) - \log(Z(w))\right] - \mathbb{E}_{Q_\theta(H|O)}\left[\sum_{r(a_r)\in H} \log Q_\theta(r(a_r))\right]$$
$$= \sum_{f\in F} w_f \sum_{a_f \in A_f} \mathbb{E}_{Q_\theta(H|O)}[\emptyset_f(a_f)] - \log(Z(w)) - \sum_{r(a_r)\in H} \mathbb{E}_{Q_\theta(H|O)}[\log Q_\theta(r(a_r))]$$

$$\mathbb{E}_{P(x)}[f(x)] = \sum_{i=1}^{I} p_i f(a_i).$$

E step: Inference

- The term $\sum_{f \in F} w_f \sum_{a_f \in A_f} \mathbb{E}_{Q_\theta(H|O)}\left[\emptyset_f\left(a_f\right)\right]$ sums over all possible logic formulae and all possible assignments to each formula
- The term $\sum_{r(a_r) \in H} \mathbb{E}_{Q_\theta(H|O)}[\log Q_\theta\left(r(a_r)\right)]$ sums over all possible latent variables
- Therefore, both terms used in the objective function make the computational problem intractable

E step: Inference with Sampling

- How can we deal with this problem?

- Do not iterate over all possible values but use sampling

  - In each optimization iteration,
    a batch of ground formulae will be sampled

  - For each formula in sampled batch, do the computations
    w.r.t. observations of involved latent variables

- $Z(w)$ needs to be adapted in order to compensate for sampling

E step: Add-on

- If the task has sufficient labeled data, a supervised learning objective will be added to enhance parameter estimation

$$L_{label}(Q_\theta) = \sum_{r(a_r) \in O} log Q_\theta(r(a_r))$$

- The label loss function is complementary to ELBO on predicates that are not well covered by logic rules but have enough observed facts

- Therefore, the E step objective function that combines knowledge in the MLN and supervision from labeled data would be (λ is a hyperparameter):

$$L_\theta = L_{ELBO}(Q_\theta, P_w) + \lambda L_{label}(Q_\theta)$$

M step: Learning

- In the M step, the weights of logic formulae in MLN will be learned with the variational posterior $Q_\theta(H|O)$ being fixed
- The partition function $Z(w)$ is not a constant anymore
- Due to exponential number of terms in $Z(w)$, pseudo log-likelihood needs to be adopted as an alternative objective for optimization
- Recall the pseudo log-likelihood

$$\log P_w(O) \approx \sum_i \log P_w\left(o_i | o_{N(i)}\right)$$

- For the neighborhood $N(i)$ we use the Markov blanket MB

Pseudo-Likelihood

$$P_w^*(O,H) \coloneqq \mathbb{E}_{Q_\theta(H|O)}\left[\sum_{r(a_r)\in H} \log P_w\big(r(a_r)|MB_{r(a_r)}\big)\right]$$

$$\nabla_{w_i}\mathbb{E}_{Q_\theta(H|O)}\left[\sum_{r(a_r)\in H} logP_w(r(a_r)|MB_{r(a_r)})\right] \simeq y_{r(a_r)} - P_w(r(a_r)|MB_{r(a_r)})$$

- where $y_{r(a_r)} = 0\ or\ 1$ if $r(a_r)$ is an observed fact or $y_{r(a_r)} = Q_\theta(r(a_r))$ otherwise
- $MB_{r(a_r)}$ is the Markov blanket of the ground predicate $r(a_r)$, i.e., the set of ground predicates that appear in some grounding of a formula with $r(a_r)$

Sampling Scheme for M step

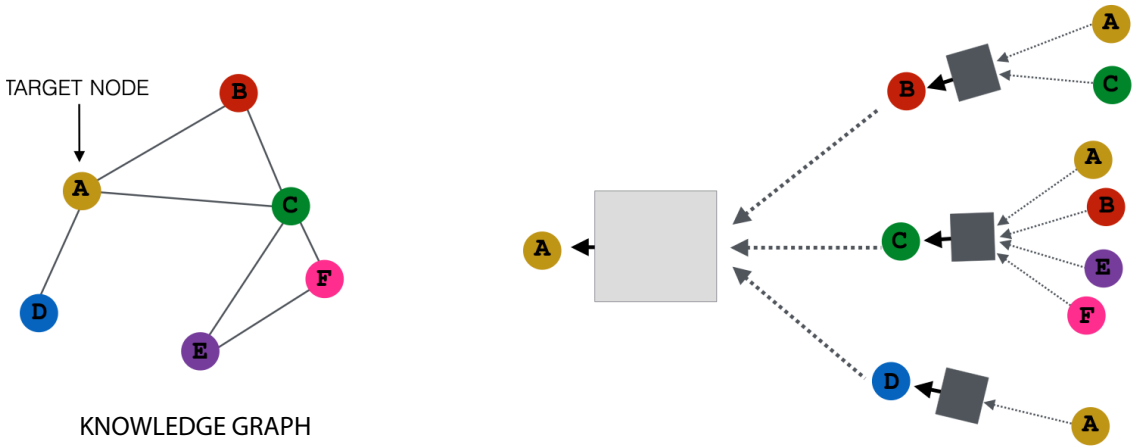
- Computationally intractable to use all possible ground predicates to compute the gradients
- The solution is to only consider all ground formulae with at most one latent predicate and pick up the ground predicate if its truth value determines the formula's truth value
- Using this sampling scheme, only a small subset of ground predicates is kept and each of which can directly determine the truth value of a ground formula in MLN
- Intuitively, this small subset contains all representative ground predicates, and makes good estimation of the gradients with much cheaper computational cost

Representing graph structures

- Foundation of MLN learning is a knowledge graph $\mathcal{G}_K$ for (deterministic) observations
- For MLN learning with hidden variables, additional graph structures need to be generated (albeit with sampling)
- Can graph structures be represented in a clever way such that we gain efficiency?
- Can we use, e.g., GNN operations to derive the variational distribution Q?

ExpressGNN

- ExpressGNN has three parts:
  - Vanilla Graph Network
  - Tunable Embeddings
  - Define posterior using embeddings



Yuyu Zhang, Xinshi Chen, Yuan Yang, Arun Ramamurthy, Bo Li, Yuan Qi & Le Song. Efficient Probabilistic Logic Reasoning with Graph Neural Networks. In: Proc. ICLR **2020**.

Vanilla GNN

- Vanilla GNN is built on knowledge graph $\mathcal{G}_K$, which is much smaller than the ground graph of MLN
  (for simplicity it is assumed that each predicate has arity 2)

- GNN parameters $\boldsymbol{\theta}_1$ and $\boldsymbol{\theta}_2$ are independent of number of entities

- There are $O(d^2)$ parameters given d-dimensional embeddings, $\mu_c \in \mathbb{R}^d$

Algorithm 1: GNN()

Initialize entity node: $\mu_c^{(0)} = \mu_0,\ \forall c \in \mathcal{C}$
for $t = 0$ *to* $T - 1$ **do**
  ▷ Compute message $\forall r(c, c') \in \mathcal{O}$
  $m_{c' \to c}^{(t)} = \mathrm{MLP}_1(\mu_{c'}^{(t)}, r; \boldsymbol{\theta}_1)$
  ▷ Aggregate message $\forall c \in \mathcal{C}$
  $m_c^{(t+1)} = \mathrm{AGG}(\{m_{c' \to c}^{(t)}\}_{c' : r(c,c') \in \mathcal{O}})$
  ▷ Update embedding $\forall c \in \mathcal{C}$
  $\mu_c^{(t+1)} = \mathrm{MLP}_2(\mu_c^{(t)}, m_c^{(t+1)}; \boldsymbol{\theta}_2)$
return embeddings $\{\mu_c^{(T)}\}$

Tunable Embeddings

- For each entity in the KG, we then augment its GNN embedding with a tunable embedding $\boldsymbol{w}_c \in \mathbb{R}^k$ as $\hat{\mu} = [\mu_c, \boldsymbol{w}_c]$
- The tunable embeddings increase the expressiveness of the model
- Otherwise, the same embeddings could be produced for nodes that should be distinguished [Zhang et al. 20]
- As there are M entities, the number of parameters in tunable embeddings is $O(kM)$

Yuyu Zhang, Xinshi Chen, Yuan Yang, Arun Ramamurthy, Bo Li, Yuan Qi & Le Song. Efficient Probabilistic Logic Reasoning with Graph Neural Networks. In: Proc. ICLR **2020**.

Define Variational Posterior

- Finally, define the variational posterior with augmented embeddings of c_1 and c_2
- Define the posterior $Q_\theta\big(r(c_1, c_2)\big) = \sigma\left(MLP_3\big(\hat{\mu}_{c_1}, \hat{\mu}_{c_2}, r; \boldsymbol{\theta}_3\big)\right)$ where $\sigma(\cdot)$ is the sigmoid function
- The number of parameters in $\boldsymbol{\theta}_3$ is $O(d + k)$

Summary so far: ExpressGNN

- In summary, ExpressGNN can be viewed as two-level encoding of entities:
  - First two MLPs assign similar embeddings to similar entities in the KG
  - Expressive tunable embeddings provide additional model capacity to encode entity information beyond graph structures
- By tuning d and k, ExpressGNN can trade-off between model **compactness** and **expressiveness**
- When the number of entities M is large, ExpressGNN can reduce k to save parameters

pLogicNet: Embeddings again

- Each entity $e \in E$ and relation $r \in R$ in a KG is associated with an embedding x_e and x_r
- The joint distribution of all triplets can be defined as:

$$p(\mathbf{v}_O, \mathbf{v}_H) = \prod_{(h,r,t) \in O \cup H} \text{Ber}\left(\mathbf{v}_{(h,r,t)} | f(\mathbf{x}_h, \mathbf{x}_r, \mathbf{x}_t)\right)$$

- Where $f(\cdot, \cdot, \cdot)$ is the scoring function on the entity and relation embeddings that computes the probability of the triplet *(h, r, t)* being true
- Example: the *f* used in TransE (a KG embedding model) is formulated as:

$$\sigma(\gamma - ||\mathbf{x}_h + \mathbf{x}_r - \mathbf{x}_t||)$$

Combining MLNs with Embedding Approaches

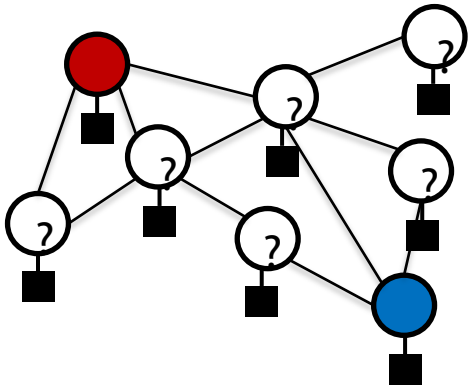
$$p_w\left(\mathbf{v}_{(h,r,t)}|\mathbf{v}_O\right) \propto \left\{ \underbrace{q_\theta\left(\mathbf{v}_{(h,r,t)}\right)}_{\text{KGE model}} + \lambda \underbrace{p_w\left(\mathbf{v}_{(h,r,t)}|\hat{\mathbf{v}}_{\mathbf{MB}(h,r,t)}\right)}_{\text{Markov Logic Network}} \right\}$$

Meng Qu and Jian Tang. Probabilistic logic neural networks for reasoning. In: Proc. NeurIPS **2019**.

MLNs w/ Node Attributes

- Model the joint distribution of the object labels given object features, i.e., $p(\mathbf{y}_V|\mathbf{x}_V)$

$$p(\mathbf{y}_V|\mathbf{x}_V) = \frac{1}{Z(\mathbf{x}_V)} \prod_{(i,j)\in E} \psi_{i,j}(\mathbf{y}_i, \mathbf{y}_j, \mathbf{x}_V)$$



Object labels

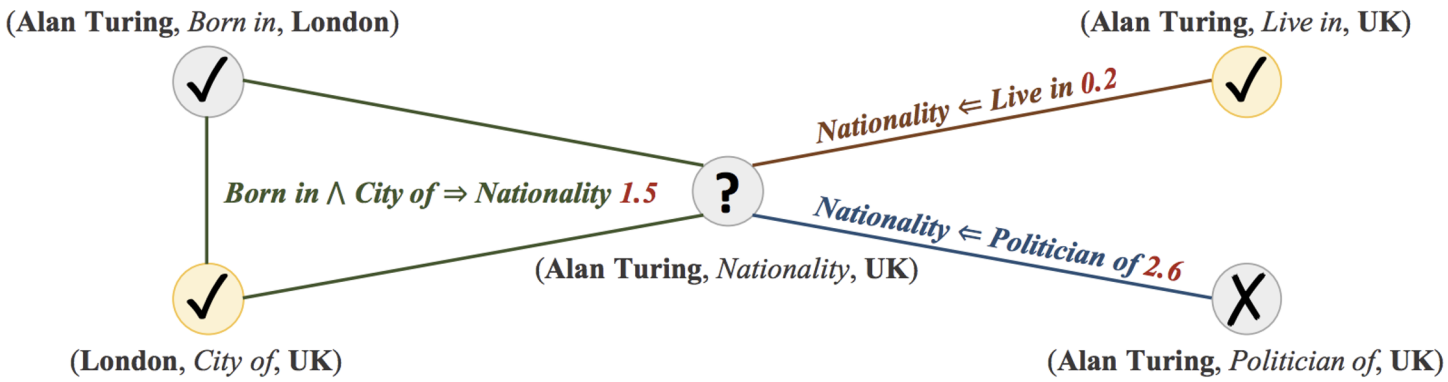
Object features

$$\psi_{i,j}(y_i, y_j, \mathbf{x}_V) = \exp\left(\sum_{k=1}^{K} \lambda_k f_k(y_i, y_j, \mathbf{x}_i, \mathbf{x}_j) + \mu_k g_k(y_i, \mathbf{x}_i)\right)$$

Edge potential functions

node potential functions

MLN Learning with pLogicNet



- pLogicNet formulates the **joint distribution of all graph triplets** with a **Markov logic network**, which is trained with the **variational EM algorithm.**

  In **E-step**, a KGE model infers missing (hidden) triplets. Knowledge preserved by logic rules can be effectively distilled into the learned embeddings.

  In **M-step**, the weights of the logic rules are updated based on both the observed triplets and those inferred by KGE model. Therefore, KGE model provides extra supervision for weight learning

Summary

- MLNs help to augment KGs
  - Constraints on graphs describe completion rules
- KGs can be used to support MLN learning
  - Embedding-based graph completion to infer missing (hidden) information, which can be used for learning
  - GNN embeddings of KG nodes for variational EM

- We can in principle combine the advantages of both worlds, logic and embedding approaches!