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# Stanford CS224W: Machine Learning with Heterogeneous Graphs

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



# Announcements

- **Colab 1** due **today**
  - Gradescope submissions close at 11:59 PM
- **Homework 1** due this Thursday

# Stanford CS224W: Heterogeneous Graphs

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

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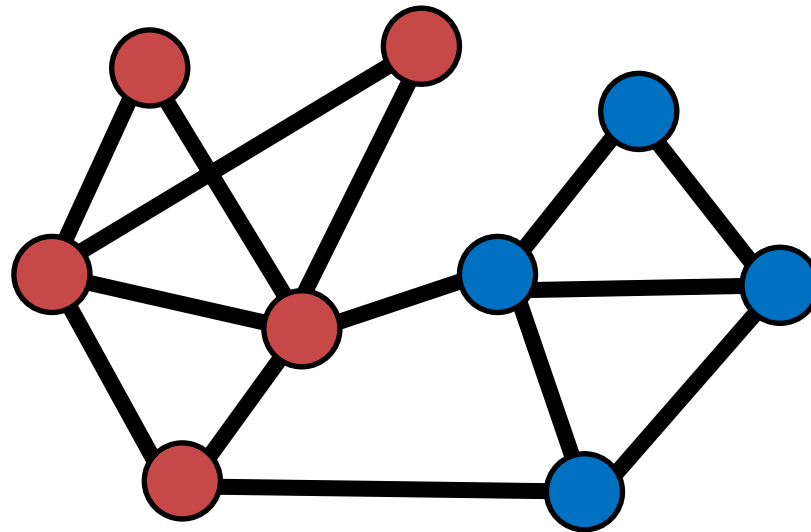


# Today: Heterogeneous Graphs

- So far we only handle graphs with one edge type
- How to handle graphs with multiple nodes or edge types (a.k.a **heterogeneous graphs**)?
- **Goal:** Learning with **heterogeneous graphs**
  - Relational GCNs
  - Heterogeneous Graph Transformer
  - **Design space for heterogeneous GNNs**



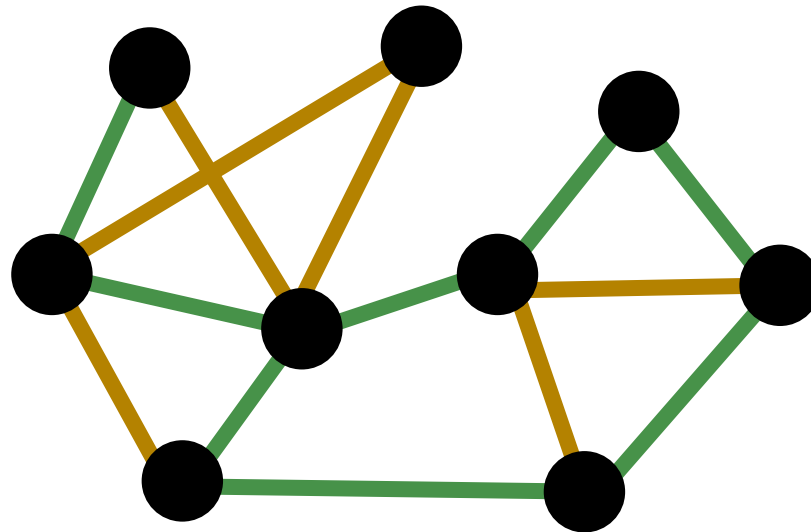
# Heterogeneous Graphs: Motivation



**2 types of nodes:**

- **Node type A:** Paper nodes
- **Node type B:** Author nodes

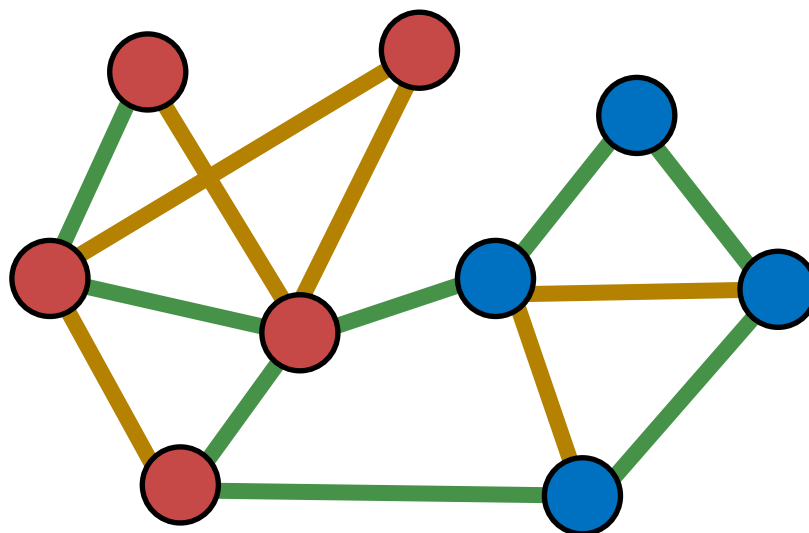
# Heterogeneous Graphs: Motivation



**2 types of edges:**

- Edge type A: Cite
- Edge type B: Like

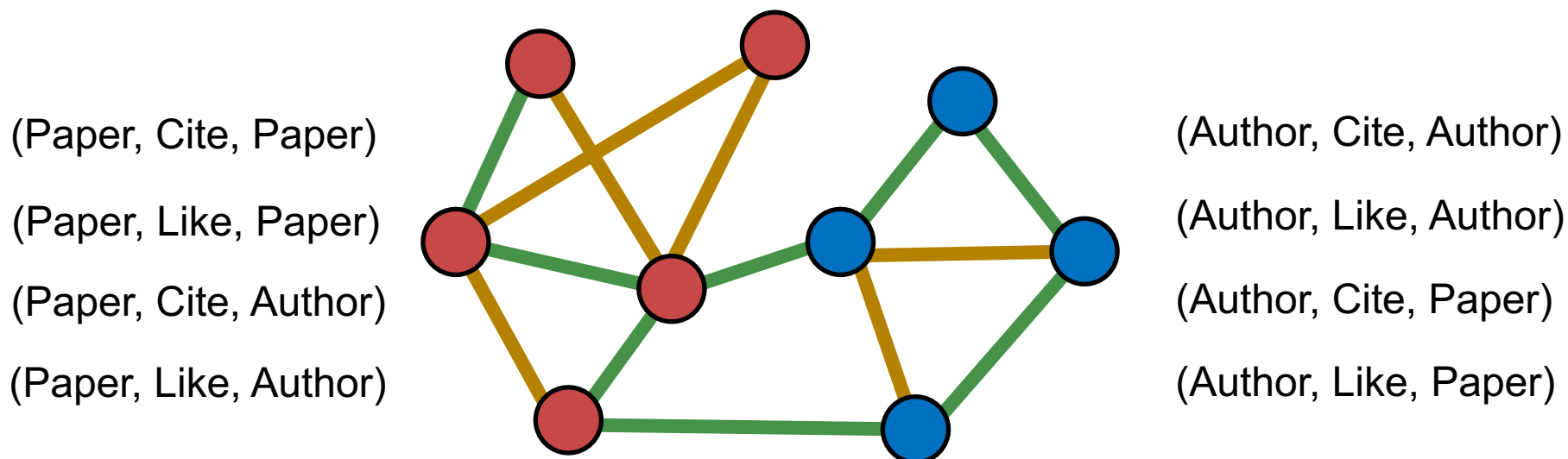
# Heterogeneous Graphs: Motivation



A graph could have multiple types of nodes and edges! **2 types of nodes + 2 types of edges.**

# Heterogeneous Graphs: Motivation

## 8 possible relation types!



**Relation types:** (node\_start, edge, node\_end)

- We use **relation type to describe an edge** (as opposed to edge type)
- Relation type better captures the interaction between nodes and edges

# Heterogeneous Graphs

- A heterogeneous graph is defined as

$$G = (V, E, \tau, \phi)$$

- Nodes with node types  $v \in V$

- **Node type** for node  $v$ :  $\tau(v)$

- Edges with edge types  $(u, v) \in E$

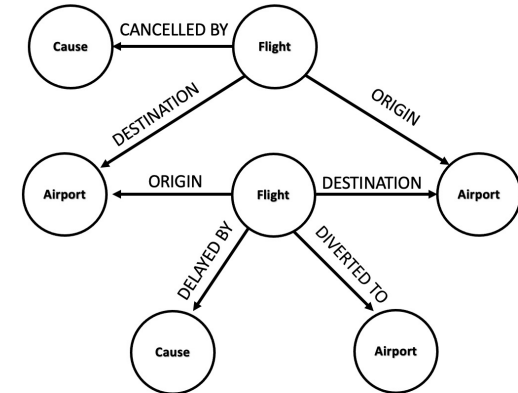
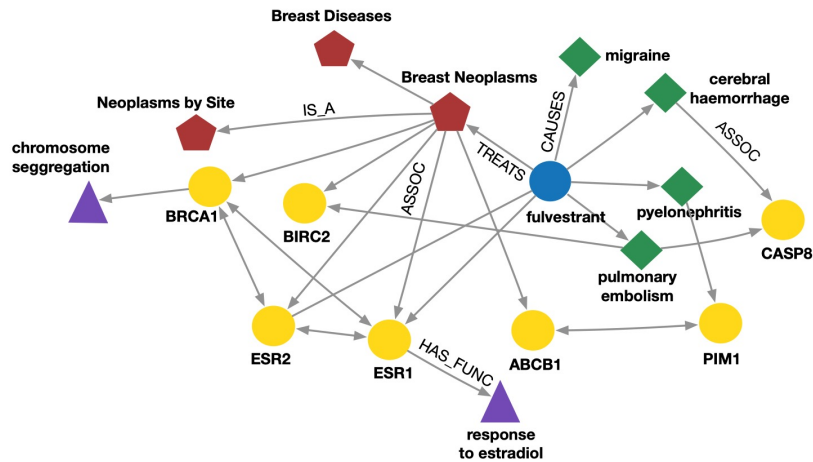
- **Edge type** for edge  $(u, v)$ :  $\phi(u, v)$

- **Relation type** for edge  $e$  is a tuple:  $r(u, v) = (\tau(u), \phi(u, v), \tau(v))$

An edge can be described as a pair of nodes

- There are other definitions for heterogeneous graphs as well – describe **graphs with node & edge types**

# Many Graphs are Heterogeneous Graphs (1)



## Biomedical Knowledge Graphs

Example node: **Migraine**

Example relation: **(fulvestrant, Treats, Breast Neoplasms)**

Example node type: **Protein**

Example edge type: **Causes**

## Event Graphs

Example node: **SFO**

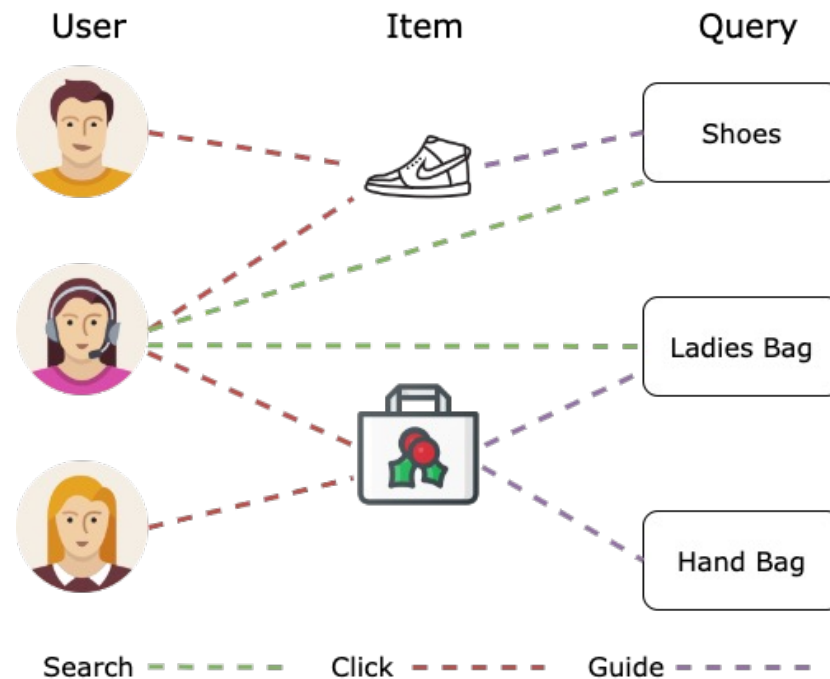
Example relation: **(UA689, Origin, LAX)**

Example node type: **Flight**

Example edge type: **Destination**

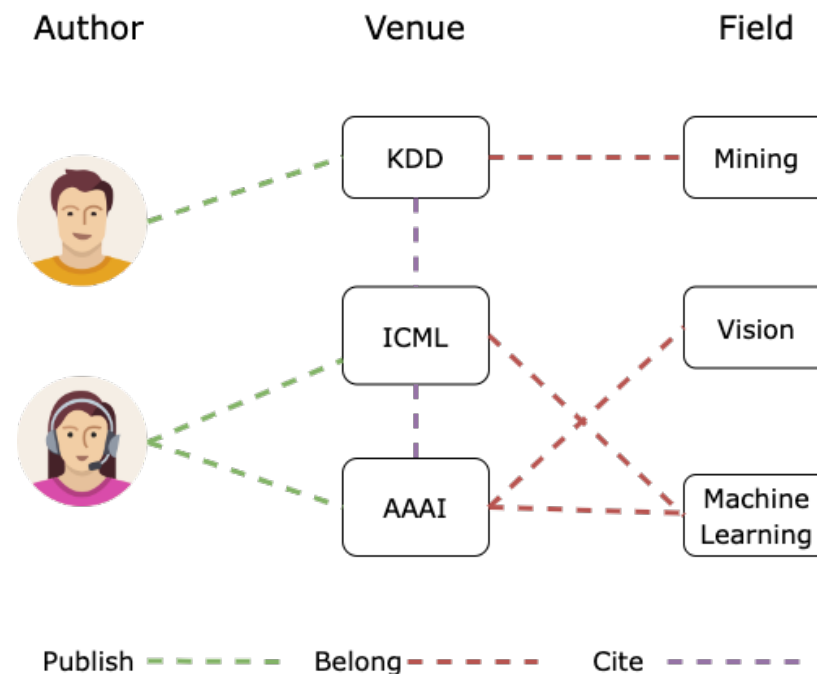
# Many Graphs are Heterogeneous Graphs (2)

- Example: E-Commerce Graph
  - **Node types:** User, Item, Query, Location, ...
  - **Edge types:** Purchase, Visit, Guide, Search, ...
  - Different node type's features spaces can be different!



# Many Graphs are Heterogeneous Graphs (3)

- Example: **Academic Graph**
  - **Node types:** Author, Paper, Venue, Field, ...
  - **Edge types:** Publish, Cite, ...
  - Benchmark dataset: **Microsoft Academic Graph**





# Discussions: Type or Feature?

- **Observation:** We can also treat types of nodes and edges as features
  - **Example:** Add a one-hot indicator for nodes and edges
    - Append feature  $[1, 0]$  to each “author node”; Append feature  $[0, 1]$  to each “paper node”
    - Similarly, we can assign edge features to edges with different types
  - Then, a heterogeneous graph reduces to a standard graph
- **When do we need a heterogeneous graph?**

# Discussions: Type or Feature?

- **When do we need a heterogeneous graph?**
  - **Case 1:** Different node/edge types **have different shapes of features**
    - An “author node” has 4-dim feature, a “paper node” has 5-dim feature
  - **Case 2:** We know different relation types represent **different types of interactions**
    - (English, translate, French) and (English, translate, Chinese) require different models

# Discussions: Heterogeneous?

- Ultimately, **heterogeneous graph is a more expressive graph representation**
  - Captures **different types of interactions between entities**
- But it also **comes with costs**
  - More expensive (computation, storage)
  - More complex implementation
- There are many ways to **convert a heterogeneous graph to a standard graph** (that is, a homogeneous graph)

# Stanford CS224W: Relational GCN (RGCN)

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



# Recap: Classical GNN Layers: GCN

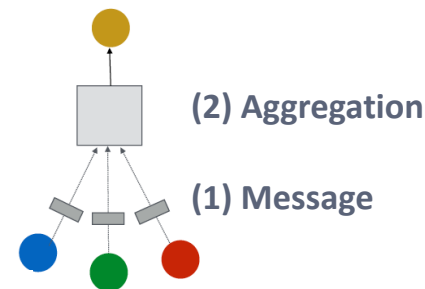
## ■ (1) Graph Convolutional Networks (GCN)

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

## ■ How to write this as Message + Aggregation?

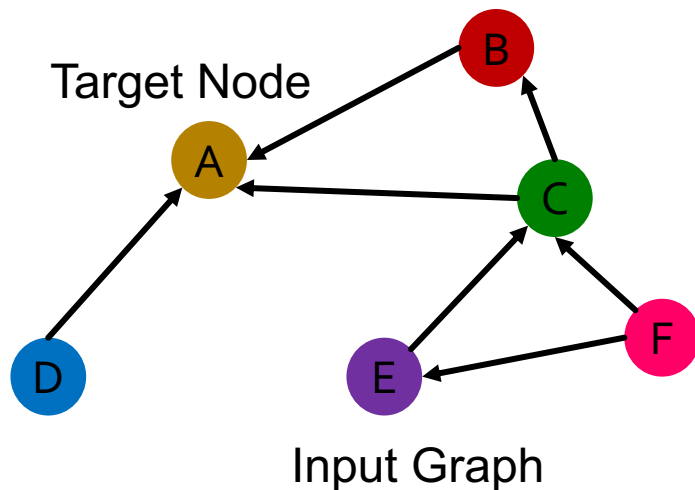
$$\mathbf{h}_v^{(l)} = \sigma \left( \underbrace{\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}}_{\text{Aggregation}} \right)$$

Message



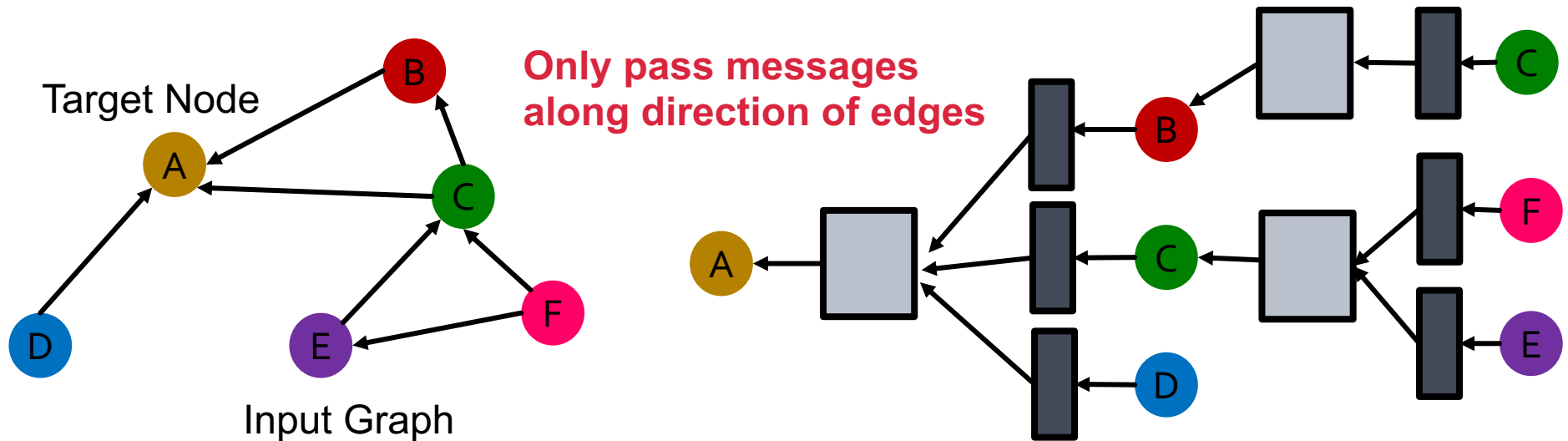
# Relational GCN

- We will extend **GCN** to handle heterogeneous graphs with multiple edge/relation types
- We start with a directed graph with **one** relation
  - How do we run GCN and update the representation of the **target node A** on this graph?



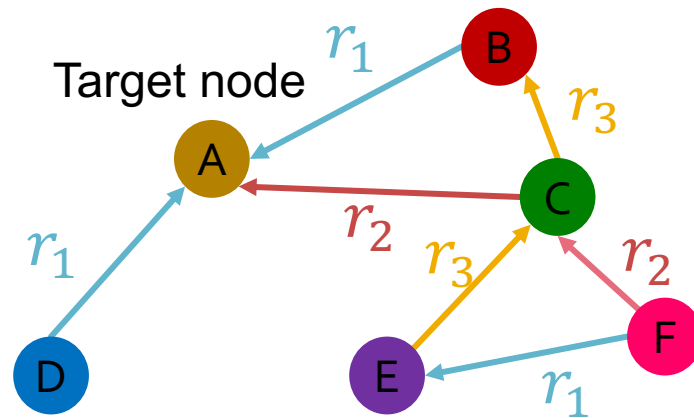
# Relational GCN

- We will extend **GCN** to handle heterogeneous graphs with multiple edge/relation types
- We start with a **directed graph** with **one** relation
  - How do we run GCN and update the representation of the **target node A** on this graph?



# Relational GCN (1)

- What if the graph has **multiple relation types**?

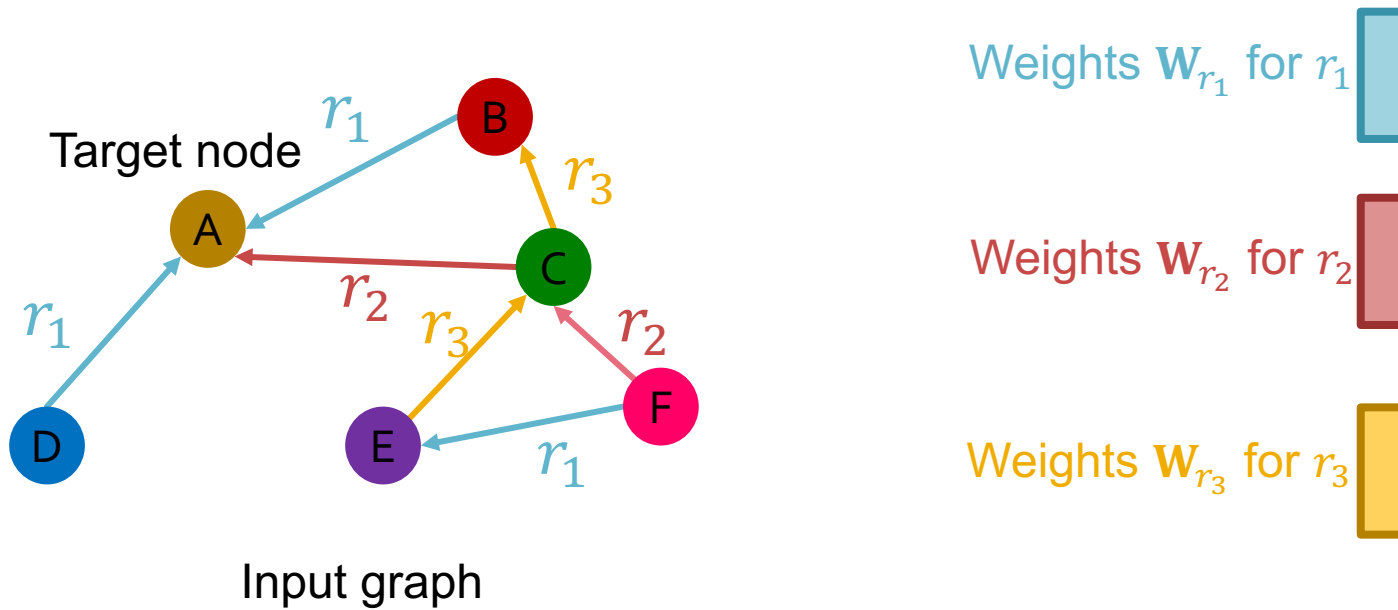


Input graph



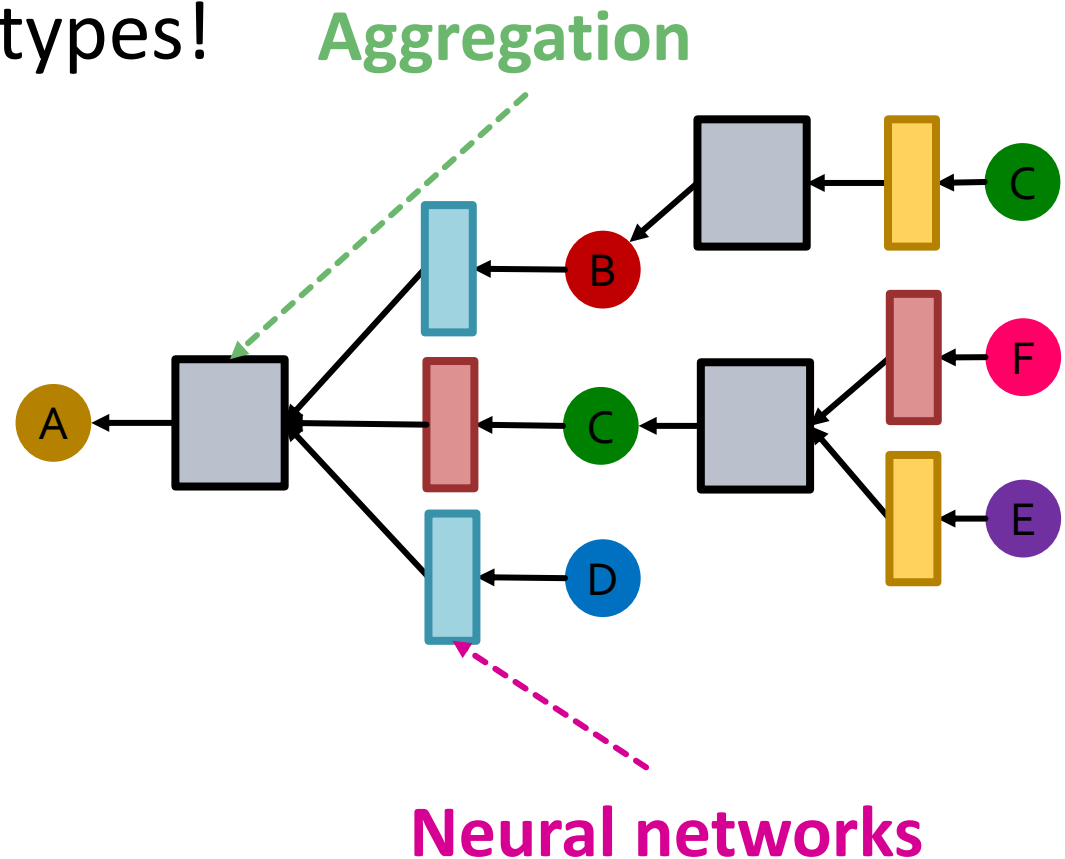
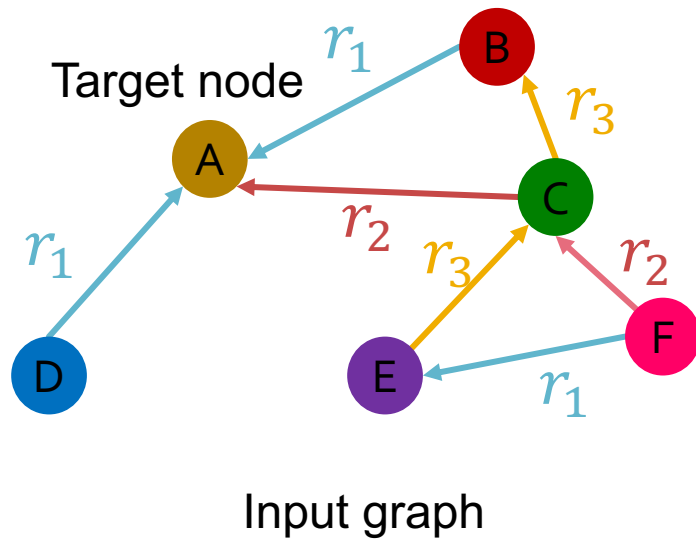
# Relational GCN (2)

- What if the graph has **multiple relation types**?
- Use different neural network weights for different relation types.



# Relational GCN (3)

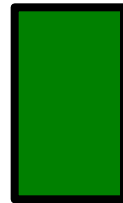
- What if the graph has **multiple relation types**?
- Use different neural network weights for different relation types!



# Relational GCN (4)

- Introduce a set of neural networks for each relation type!

Weight for rel\_1

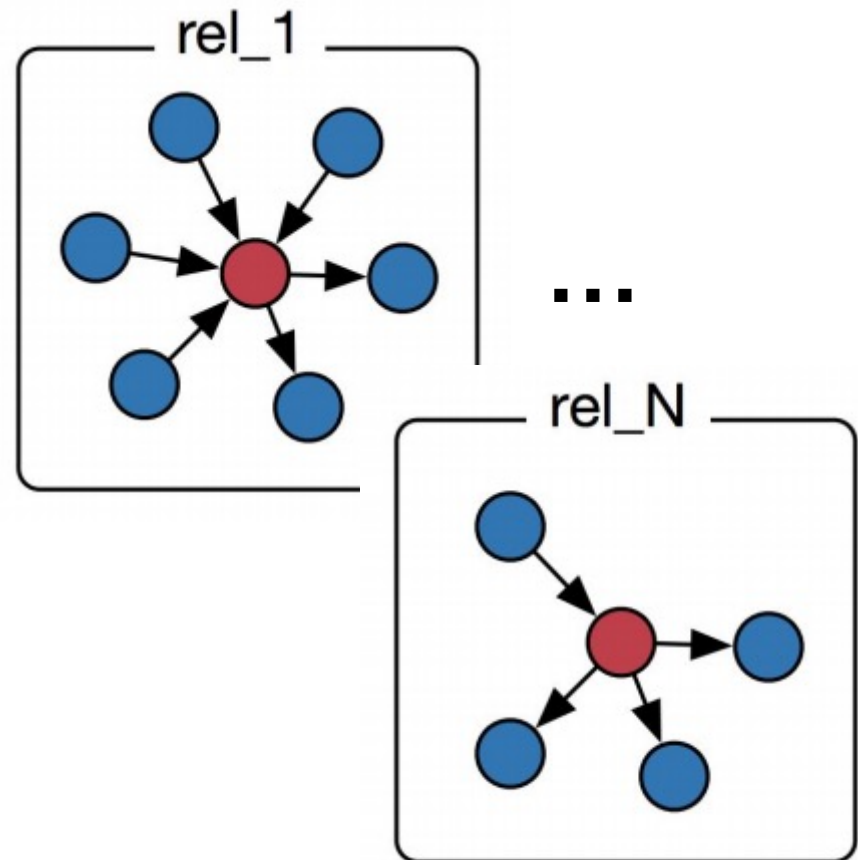
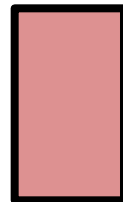


...

Weight for rel\_N



Weight for self-loop



# Relational GCN: Definition

- **Relational GCN (RGCN):**

$$\mathbf{h}_v^{(l+1)} = \sigma \left( \sum_{r \in R} \sum_{u \in N_v^r} \frac{1}{c_{v,r}} \mathbf{W}_r^{(l)} \mathbf{h}_u^{(l)} + \mathbf{W}_0^{(l)} \mathbf{h}_v^{(l)} \right)$$

- **How to write this as Message + Aggregation?**

- **Message:**

Normalized by node degree of the relation  $c_{v,r} = |N_v^r|$

- Each neighbor of a given relation:

$$\mathbf{m}_{u,r}^{(l)} = \frac{1}{c_{v,r}} \mathbf{W}_r^{(l)} \mathbf{h}_u^{(l)}$$

- Self-loop:

$$\mathbf{m}_v^{(l)} = \mathbf{W}_0^{(l)} \mathbf{h}_v^{(l)}$$

- **Aggregation:**

- Sum over messages from neighbors and self-loop, then apply activation

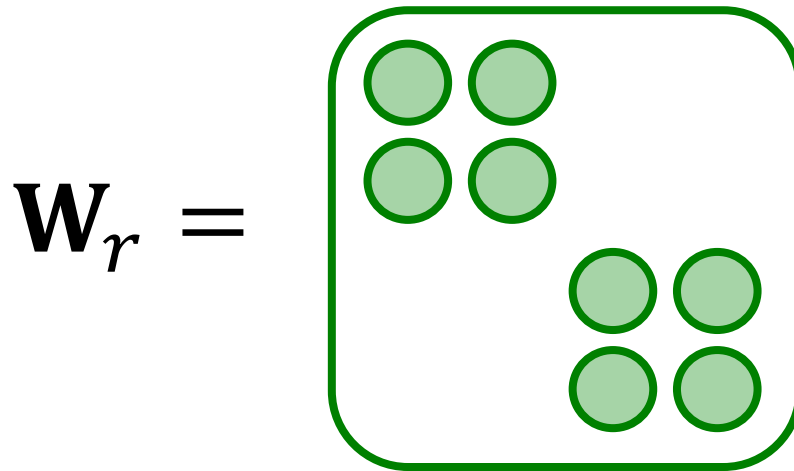
- $\mathbf{h}_v^{(l+1)} = \sigma \left( \text{Sum} \left( \left\{ \mathbf{m}_{u,r}^{(l)}, u \in N(v) \right\} \cup \left\{ \mathbf{m}_v^{(l)} \right\} \right) \right)$

# RGCN: Scalability

- Each relation has  $L$  matrices:  $\mathbf{W}_r^{(1)}, \mathbf{W}_r^{(2)} \dots \mathbf{W}_r^{(L)}$
- The size of each  $\mathbf{W}_r^{(l)}$  is  $d^{(l+1)} \times d^{(l)}$   $d^{(l)}$  is the hidden dimension in layer  $l$
- **Rapid growth of the number of parameters w.r.t number of relations!**
  - **Overfitting becomes an issue**
- **Two methods to regularize the weights  $\mathbf{W}_r^{(l)}$** 
  - **(1)** Use block diagonal matrices
  - **(2)** Basis/Dictionary learning

# (1) Block Diagonal Matrices

- **Key insight:** make the weights **sparse**!
- Use **block diagonal matrices** for  $\mathbf{W}_r$



**Limitation:** only nearby neurons/dimensions can interact through  $W$

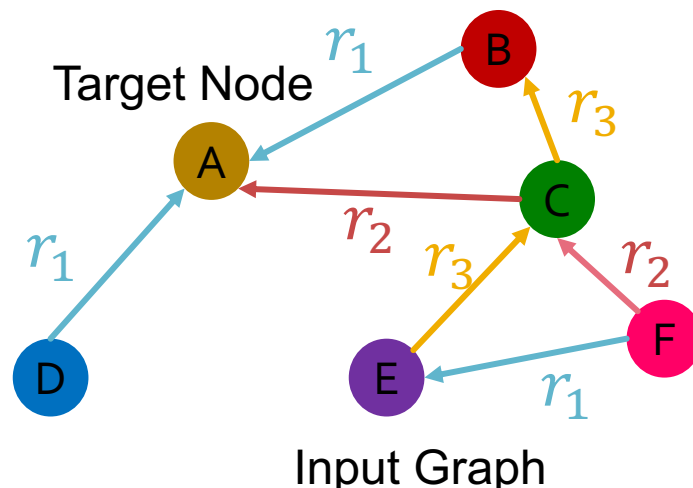
- If use  $B$  low-dimensional matrices, then # param reduces from  $d^{(l+1)} \times d^{(l)}$  to  $B \times \frac{d^{(l+1)}}{B} \times \frac{d^{(l)}}{B}$

## (2) Basis Learning

- **Key insight: Share weights** across different relations!
- Represent the matrix of each relation as a **linear combination** of **basis transformations**  
 $\mathbf{W}_r = \sum_{b=1}^B a_{rb} \cdot \mathbf{V}_b$ , where  $\mathbf{V}_b$  is shared across all relations
  - $\mathbf{V}_b$  are the basis matrices
  - $a_{rb}$  is the importance weight of matrix  $\mathbf{V}_b$
- Now each relation only needs to learn  $\{a_{rb}\}_{b=1}^B$ , which is  $B$  scalars

# Example: Entity/Node Classification

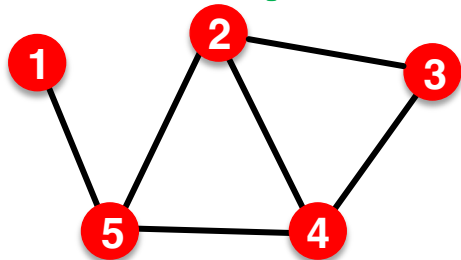
- **Goal:** Predict the label of a given node
- **RGCN** uses the representation of the final layer:
  - If we predict the class of **node A** from  **$k$  classes**
  - Take the **final layer (prediction head)**:  $\mathbf{h}_A^{(L)} \in \mathbb{R}^k$ , each item in  $\mathbf{h}_A^{(L)}$  represents **the probability of that class**





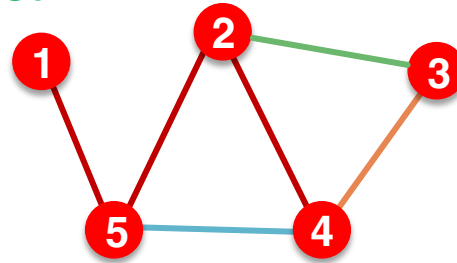
# Example: Link Prediction

## ■ Link prediction split:



The original graph

Split  
→



Split Graph with 4 categories of edges

Every edge also has a relation type, this is independent of the 4 categories.

In a heterogeneous graph, the homogeneous graphs formed by every single relation also have the 4 splits.

Training message edges for  $r_1$   
Training supervision edges for  $r_1$   
Validation edges for  $r_1$   
Test edges for  $r_1$

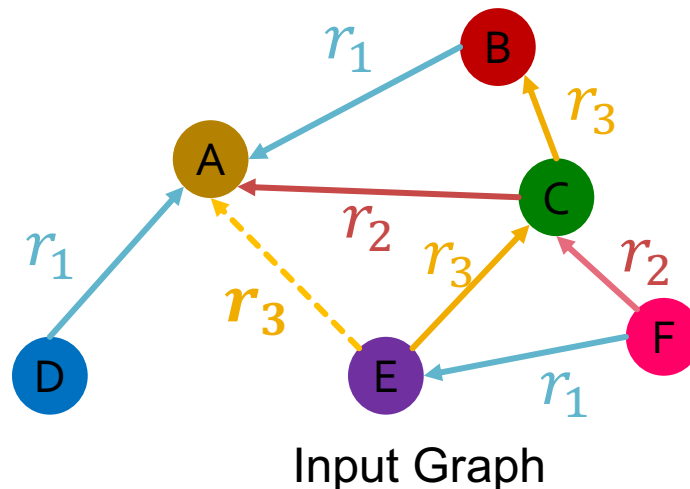
⋮

Training message edges for  $r_n$   
Training supervision edges for  $r_n$   
Validation edges for  $r_n$   
Test edges for  $r_n$

Training message edges  
Training supervision edges  
Validation edges  
Test edges

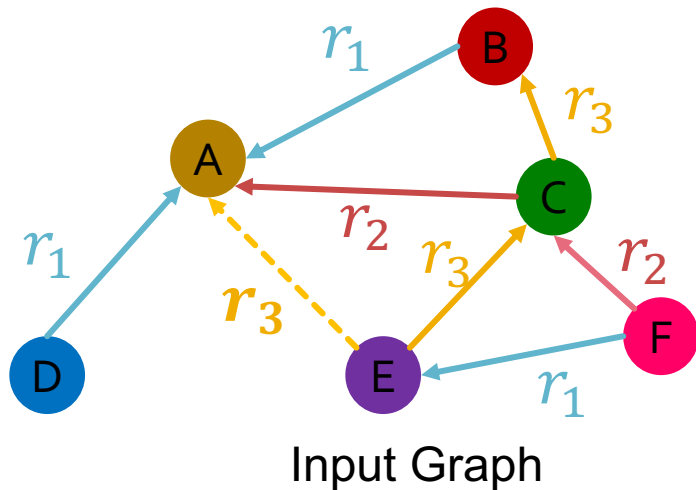
# RGCN for Link Prediction (1)

- Assume  $(E, r_3, A)$  is training supervision edge, all the other edges are training message edges
- Use RGCN to score  $(E, r_3, A)$ !
  - Take the final layer of  $E$  and  $A$ :  $\mathbf{h}_E^{(L)}$  and  $\mathbf{h}_A^{(L)} \in \mathbb{R}^d$
  - Relation-specific score function  $f_r: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ 
    - One example  $f_{r_1}(\mathbf{h}_E, \mathbf{h}_A) = \mathbf{h}_E^T \mathbf{W}_{r_1} \mathbf{h}_A$ ,  $\mathbf{W}_{r_1} \in \mathbb{R}^{d \times d}$



# RGCN for Link Prediction (2)

## ■ Training:



1. Use RGCN to score the **training supervision edge**  $(E, r_3, A)$
2. Create a **negative edge** by perturbing the **supervision edge**  $(E, r_3, B)$ 
  - Corrupt the **tail** of  $(E, r_3, A)$ 
    - e.g.,  $(E, r_3, B)$ ,  $(E, r_3, D)$

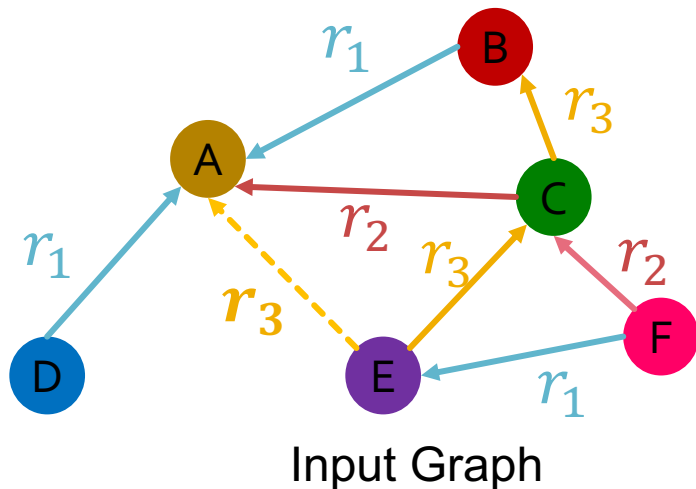
**training supervision edges:**  $(E, r_3, A)$   
**training message edges:** all the rest existing edges (solid lines)

**Note the negative edges should NOT belong to training message edges or training supervision edges!**  
e.g.,  $(E, r_3, C)$  is **NOT** a **negative edge**

(1) Use **training message edges** to predict **training supervision edges**

# RGCN for Link Prediction (3)

## ■ Training:



1. Use RGCN to score the **training supervision edge** ( $E, r_3, A$ )
2. Create a **negative edge** by perturbing the **supervision edge** ( $E, r_3, B$ )
3. Use GNN model to score **negative edge**
4. Optimize a standard cross entropy loss (as discussed in Lecture 6)
  1. **Maximize** the score of **training supervision edge**
  2. **Minimize** the score of **negative edge**

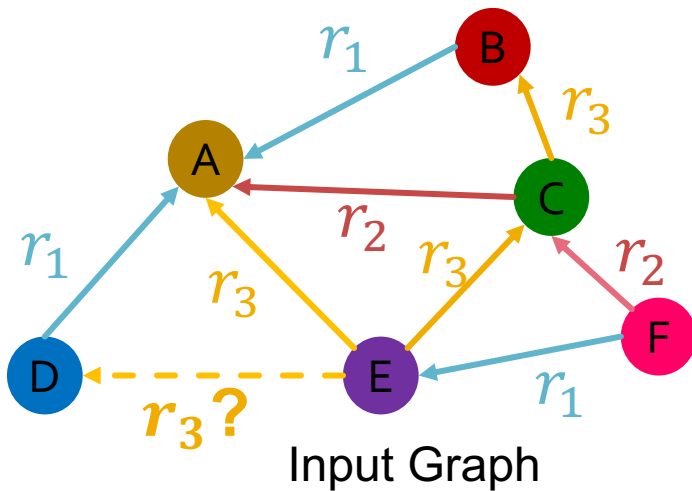
$$\ell = -\log \sigma \left( f_{r_3}(h_E, h_A) \right) - \log(1 - \sigma(f_{r_3}(h_E, h_B)))$$

$\sigma$  ... Sigmoid function

# RGCN for Link Prediction (4)

## ■ Evaluation:

- Validation time as an example, same at the test time



Evaluate how the model can predict the validation edges with the relation types.

Let's predict validation edge  $(E, r_3, D)$

**Intuition:** the score of  $(E, r_3, D)$  should be higher than all  $(E, r_3, v)$  where  $(E, r_3, v)$  is **NOT** in the **training message edges** and **training supervision edges**, e.g.,  $(E, r_3, B)$

validation edges:  $(E, r_3, D)$

training message edges & training supervision

edges: all existing edges (solid lines)

(2) At validation time:

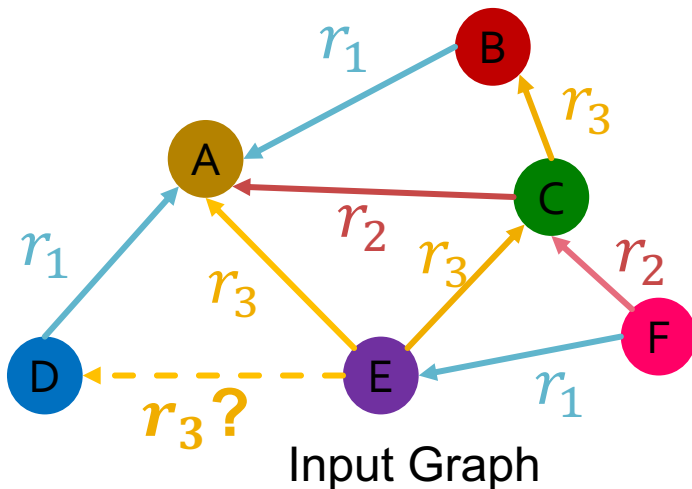
Use **training message edges & training**

**supervision edges** to predict **validation edges**

# RGCN for Link Prediction (5)

## ■ Evaluation:

- Validation time as an example, same at the test time



Evaluate how the model can predict the validation edges with the relation types.

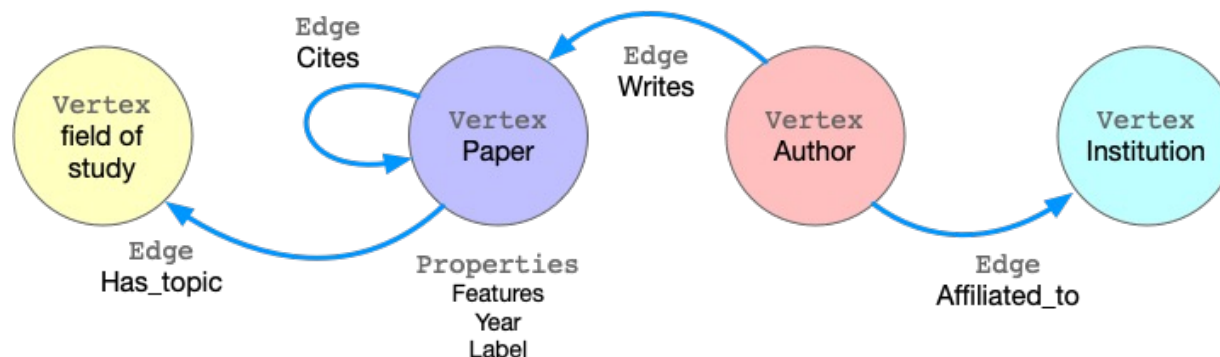
Let's predict validation edge  $(E, r_3, D)$

**Intuition:** the score of  $(E, r_3, D)$  should be higher than all  $(E, r_3, v)$  where  $(E, r_3, v)$  is **NOT** in the **training message edges** and **training supervision edges**, e.g.,  $(E, r_3, B)$

1. Calculate the score of  $(E, r_3, D)$
2. Calculate the score of all the negative edges:  $\{(E, r_3, v) | v \in \{B, F\}\}$ , since  $(E, r_3, A)$ ,  $(E, r_3, C)$  belong to **training message edges & training supervision edges**
3. Obtain the ranking  $RK$  of  $(E, r_3, D)$ .
4. Calculate metrics
  1. Hits@ $k$ :  $1 [RK \leq k]$ . Higher is better
  2. Reciprocal Rank:  $\frac{1}{RK}$ . Higher is better

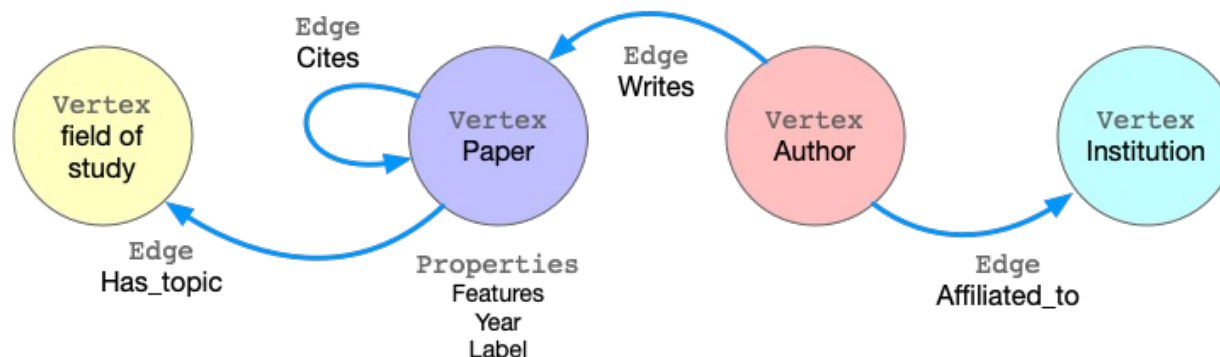
# Benchmark for Heterogeneous Graphs (1)

- Benchmark dataset
  - [ogbn-mag](#) from Microsoft Academic Graph (MAG)
- Four (4) **types of entities**
  - **Papers**: 736k nodes
  - **Authors**: 1.1m nodes
  - **Institutions**: 9k nodes
  - **Fields of study**: 60k nodes



# Benchmark for Heterogeneous Graphs (2)

- Benchmark dataset
  - [ogbn-mag](#) from Microsoft Academic Graph (MAG)
- Four (4) **directed relations**
  - An **author** is "affiliated with" an **institution**
  - An **author** "writes" a **paper**
  - A **paper** "cites" a **paper**
  - A **paper** "has a topic of" a **field of study**





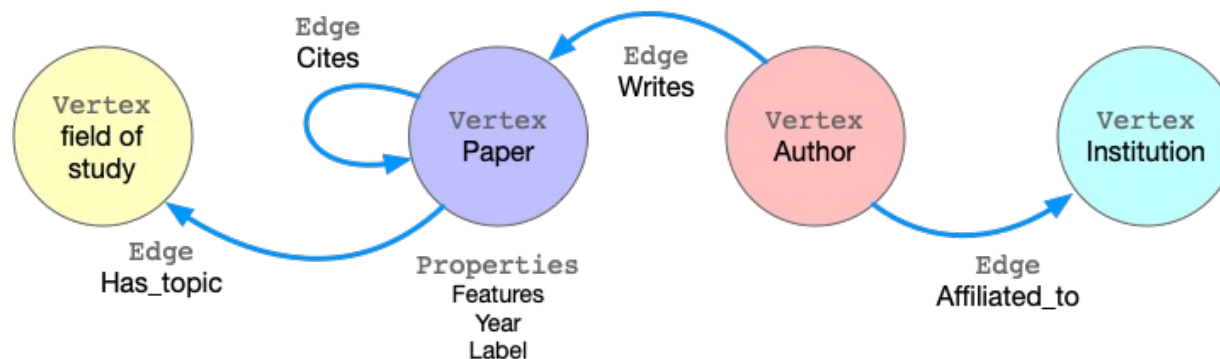
# Benchmark for Heterogeneous Graphs (3)

## ■ Prediction task

- Each paper has a **128-dimensional word2vec** feature vector
- Given the **content, references, authors, and author affiliations** from ogbn-mag, predict the **venue of each paper**
- **349-class** classification problem due to 349 venues considered

## ■ Time-based dataset splitting

- **Training set:** papers published **before 2018**
- **Test set:** papers published **after 2018**



# Benchmark for Heterogeneous Graphs (4)

## ■ Benchmark results:

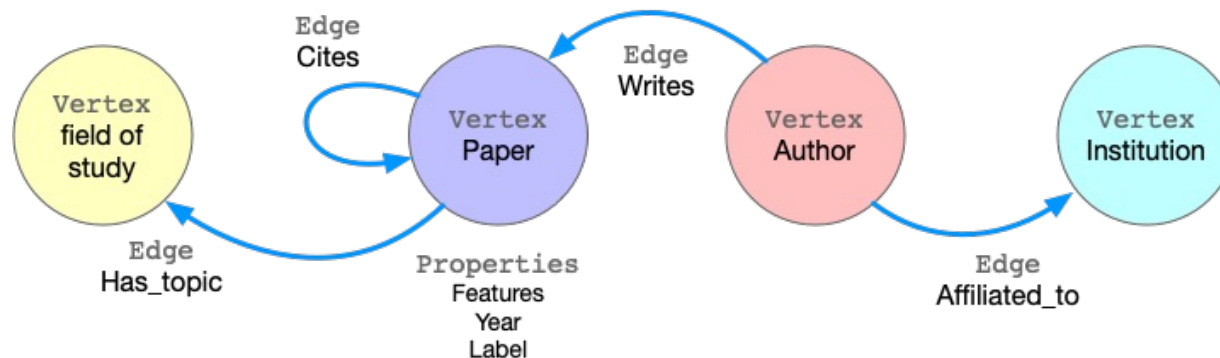
Rank	Method	Ext. data	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
1	SeHGNN (Complex embs)	No	0.5719 ± 0.0012	0.5917 ± 0.0009	<a href="#">Xiaocheng Yang (ICT-GIMLab)</a>	<a href="#">Paper</a> , <a href="#">Code</a>	8,371,231	NVIDIA Tesla T4 (15 GB)	Jul 7, 2022
21	NeighborSampling (R-GCN aggr)	No	0.4678 ± 0.0067	0.4761 ± 0.0068	<a href="#">Matthias Fey – OGB team</a>	<a href="#">Paper</a> , <a href="#">Code</a>	154,366,772	GeForce RTX 2080 (11GB GPU)	Jun 26, 2020

SOTA

R-GCN

## ■ SOTA method: SeHGNN

- Complex (Next lecture) + Simplified GCN (Lecture 17)



# Summary of RGCN

- **Relational GCN**, a graph neural network for heterogeneous graphs
- Can perform entity classification as well as link prediction tasks.
- Ideas can easily be extended into RGNN (RGraphSAGE, RGAT, etc.)
- **Benchmark:** [ogbn-mag](#) from Microsoft Academic Graph, to predict **paper venues**

# Stanford CS224W: Heterogeneous Graph Transformer

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



# Recap: Graph Attention Networks

## ■ Graph Attention Networks (GAT)

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \alpha_{vu} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

Attention weights

## Not all node's neighbors are equally important

- **Attention** is inspired by cognitive attention.
- The **attention**  $\alpha_{vu}$  focuses on the important parts of the input data and fades out the rest.
  - **Idea:** the NN should devote more computing power on that small but important part of the data.
- **Can we adapt GAT for heterogeneous graphs?**

# Heterogeneous Graph Transformer

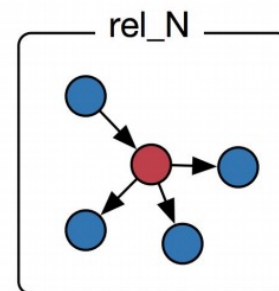
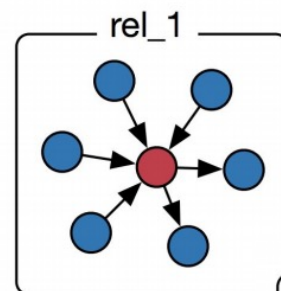
- **Motivation:** GAT is **unable to represent** different node & different edge types
- Introduce a set of neural networks for each relation type is **too expensive** for attention
  - **Recall:** relation describes (node\_s, edge, node\_e)

Weight for rel\_1



...

Weight for rel\_N



**Too expensive!**

# Basics: Attention in Transformer

- HGT uses Scaled Dot-Product Attention (proposed in Transformer)

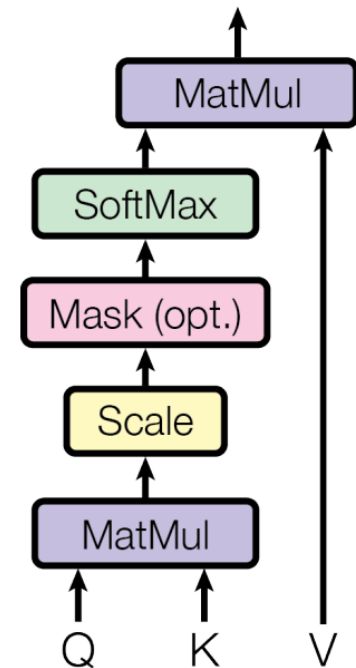
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

Scaled Dot-Product Attention

- Query:  $Q$ , Key:  $K$ , Value:  $V$ 
  - $Q, K, V$  have shape (batch\_size, dim)

How do we obtain  $Q, K, V$ ?

- Apply Linear layer to the input
  - $Q = Q\_Linear(X)$
  - $K = K\_Linear(X)$
  - $V = V\_Linear(X)$

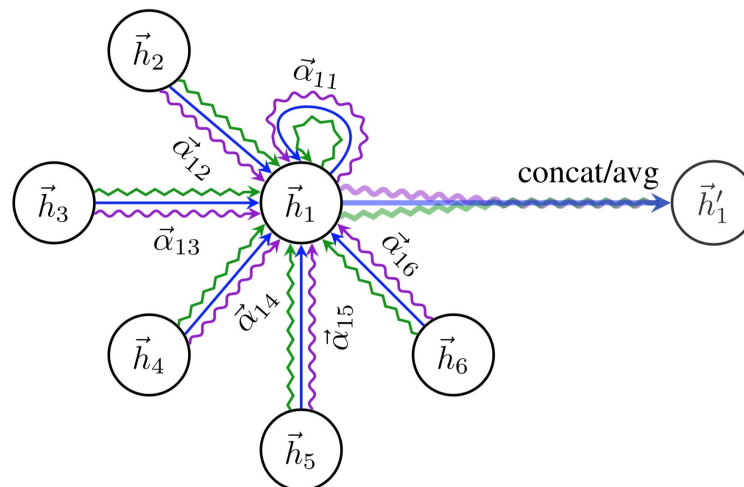


# Heterogeneous Mutual Attention (1)

- **Recall:** Applying GAT to a homogeneous graph
  - $H^{(l)}$  is the  $l$ -th layer representation:

$$H^l[t] \leftarrow \text{Aggregate}_{\forall s \in N(t), \forall e \in E(s,t)} \boxed{\text{Attention}(s, t)} \cdot \text{Message}(s)$$

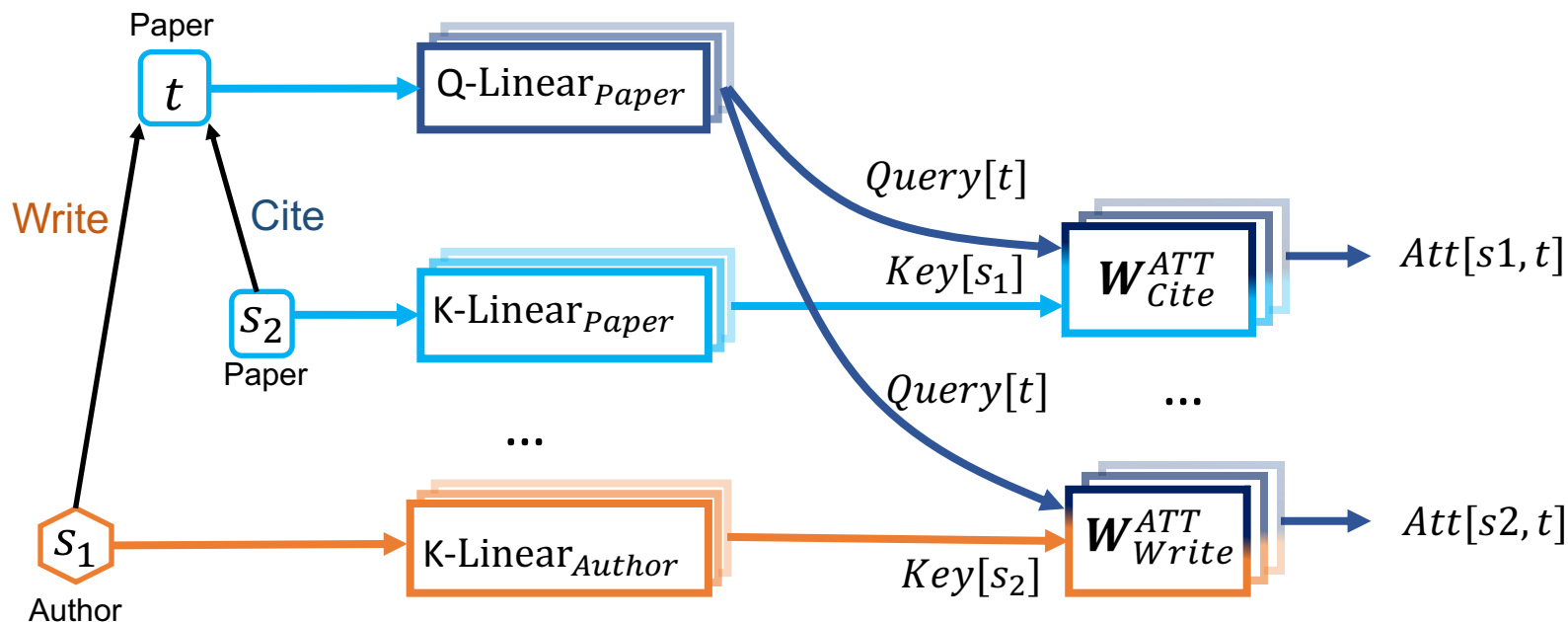
How do we take relation type (node\_s, edge, node\_e) into attention computation?





# Heterogeneous Mutual Attention (2)

- Innovation:** Decompose heterogeneous attention to **Node- and edge-type dependent attention mechanism**
  - 3 node weight matrices, 2 edge weight matrices**
  - Without decomposition:**  $3 \times 2 \times 3 = 18$  relation types  $\rightarrow$  18 weight matrices (suppose all relation types exist)



# Heterogeneous Mutual Attention (3)

- **Heterogeneous Mutual Attention:**

$$ATT-head^i(s, e, t) = \left( K^i(s) W_{\phi(e)}^{ATT} Q^i(t)^T \right)$$

$$K^i(s) = \text{K-Linear}_{\tau(s)}^i \left( H^{(l-1)}[s] \right)$$

$$Q^i(t) = \text{Q-Linear}_{\tau(t)}^i \left( H^{(l-1)}[t] \right)$$

- Each **relation**  $(T(s), R(e), T(t))$  has a distinct set of **projection weights**
  - $T(s)$ : type of node  $s$ ,  $R(e)$ : type of edge  $e$
  - $T(s)$  &  $T(t)$  parameterize  $K\_Linear_{T(s)}$  &  $Q\_Linear_{T(t)}$ , which further return Key and Query vectors  $K(s)$  &  $Q(t)$
  - Edge type  $R(e)$  directly parameterizes  $W_{R(e)}$

# More Details on HGT

- A full HGT layer

$$\tilde{H}^{(l)}[t] = \bigoplus_{\forall s \in N(t)} \left( \text{Attention}_{HGT}(s, e, t) \cdot \text{Message}_{HGT}(s, e, t) \right)$$

**We have just computed**

- Similarly, HGT decomposes weights with node & edge types in the message computation

$$\text{Message}_{HGT}(s, e, t) = \parallel_{i \in [1, h]} \text{MSG-head}^i(s, e, t)$$

$$\text{MSG-head}^i(s, e, t) = \text{M-Linear}_{\tau(s)}^i \left( H^{(l-1)}[s] \right) W_{\phi(e)}^{MSG}$$

**Weights for  
each node type**

**Weights for  
each edge type**

# HGT vs R-GCN: Performance

- **Benchmark: [ogbn-mag](#)** from Microsoft Academic Graph, to predict **paper venues**

Rank	Method	Ext. data	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
18	HGT (LADIES Sample)	No	0.4927 ± 0.0061	0.4989 ± 0.0047	<a href="#">Ziniu Hu</a>	<a href="#">Paper</a> , <a href="#">Code</a>	21,173,389	Tesla K80 (12GB GPU)	Jan 26, 2021
21	NeighborSampling (R-GCN aggr)	No	0.4678 ± 0.0067	0.4761 ± 0.0068	<a href="#">Matthias Fey – OGB team</a>	<a href="#">Paper</a> , <a href="#">Code</a>	154,366,772	GeForce RTX 2080 (11GB GPU)	Jun 26, 2020

- HGT uses **much fewer parameters**, even though the attention computation is expensive, while **performs better than R-GCN**
  - Thanks to the weight decomposition over node & edge types

# Stanford CS224W: Design Space of Heterogeneous GNNs

CS224W: Machine Learning with Graphs

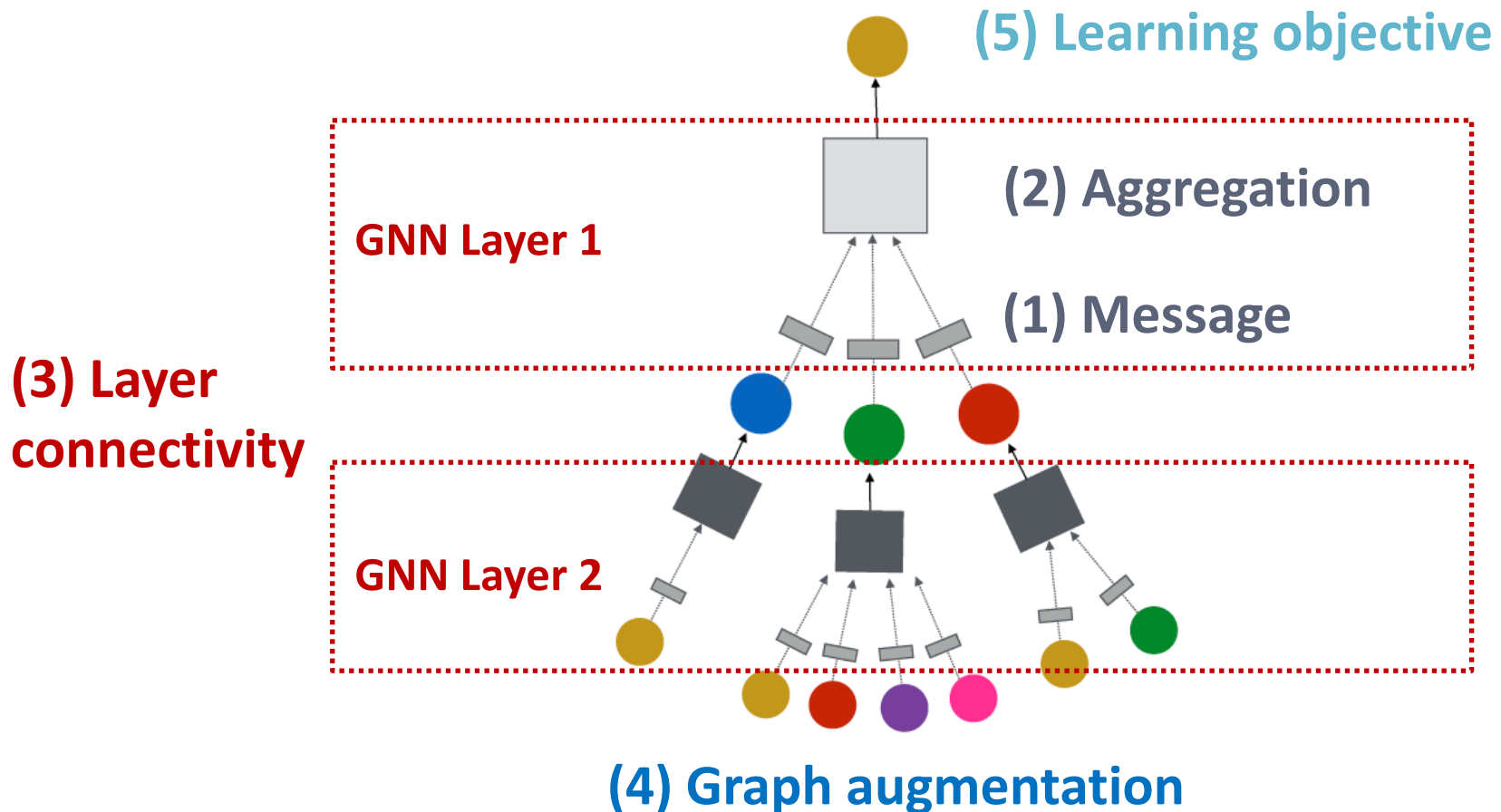
Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



# Recap: GNN Framework

How do we extend the general GNN design space to heterogeneous graphs?



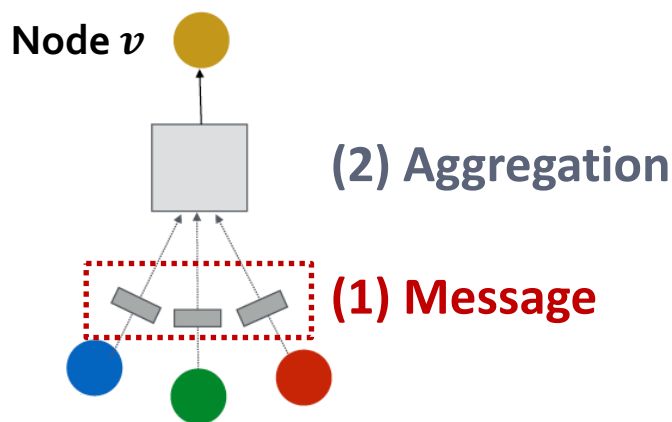
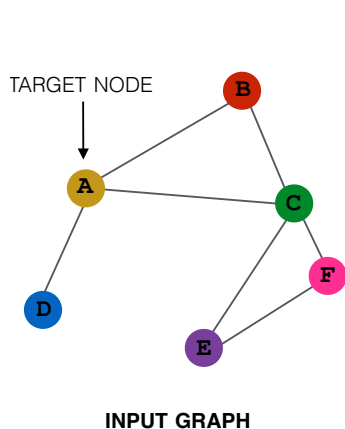
# Recap: Message Computation

## ■ (1) Message computation

■ **Message function:**  $\mathbf{m}_u^{(l)} = \text{MSG}^{(l)} \left( \mathbf{h}_u^{(l-1)} \right)$

■ **Intuition:** Each node will create a message, which will be sent to other nodes later

■ **Example:** A Linear layer  $\mathbf{m}_u^{(l)} = \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}$



# Heterogeneous Message

- **(1) Heterogeneous message computation**

- **Message function:**  $\mathbf{m}_u^{(l)} = \text{MSG}_r^{(l)} \left( \mathbf{h}_u^{(l-1)} \right)$

- **Observation:** A node could **receive multiple types of messages**. **Num of message type = Num of relation type**

- **Idea:** Create a different message function for each relation type

- $\mathbf{m}_u^{(l)} = \text{MSG}_r^{(l)} \left( \mathbf{h}_u^{(l-1)} \right)$ ,  $r = (u, e, v)$  is the relation type between node  $u$  that sends the message, edge type  $e$ , and node  $v$  that receive the message

- **Example:** A Linear layer  $\mathbf{m}_u^{(l)} = \mathbf{W}_r^{(l)} \mathbf{h}_u^{(l-1)}$



# Recap: Message Aggregation

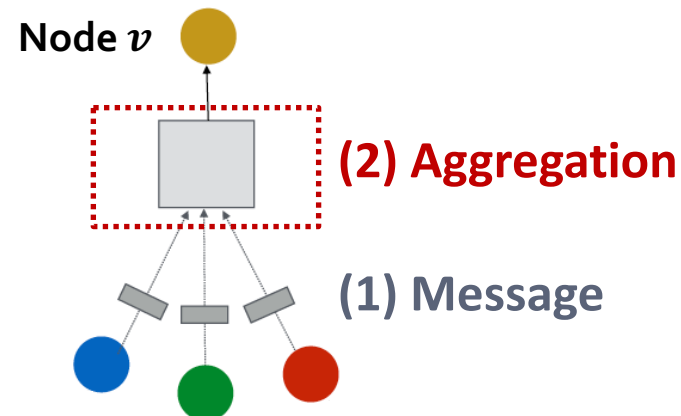
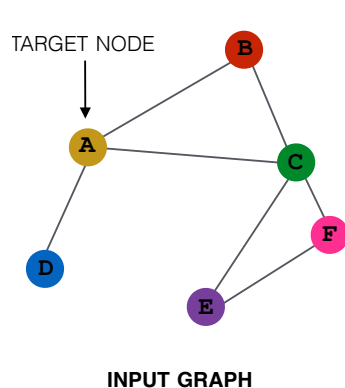
## ■ (2) Aggregation

- **Intuition:** Each node will aggregate the messages from node  $v$ 's neighbors

$$\mathbf{h}_v^{(l)} = \text{AGG}^{(l)} \left( \left\{ \mathbf{m}_u^{(l)}, u \in N(v) \right\} \right)$$

- **Example:** Sum( $\cdot$ ), Mean( $\cdot$ ) or Max( $\cdot$ ) aggregator

- $\mathbf{h}_v^{(l)} = \text{Sum}(\{\mathbf{m}_u^{(l)}, u \in N(v)\})$



# Heterogeneous Aggregation

## ■ (2) Heterogeneous Aggregation

- **Observation:** Each node could receive multiple types of messages from its neighbors, and multiple neighbors may belong to each message type.
- **Idea:** We can define a 2-stage message passing

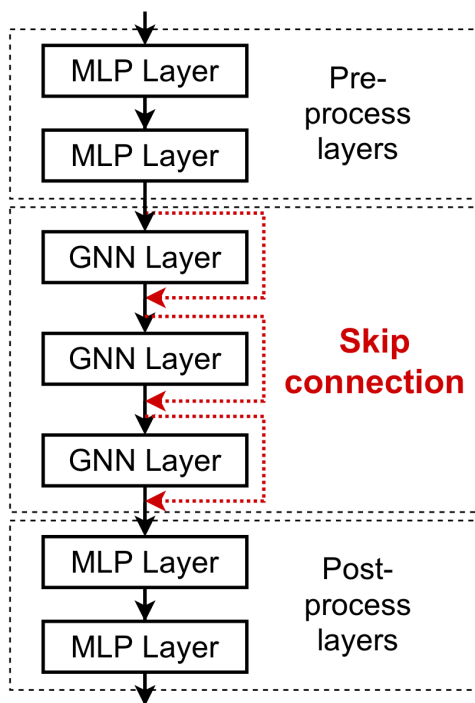
- $\mathbf{h}_v^{(l)} = \text{AGG}_{all}^{(l)} \left( \text{AGG}_r^{(l)} \left( \left\{ \mathbf{m}_u^{(l)}, u \in N_r(v) \right\} \right) \right)$

- Given all the messages sent to a node
- Within each message type, aggregate the messages that belongs to the edge type with  $\text{AGG}_r^{(l)}$
- Aggregate across the edge types with  $\text{AGG}_{all}^{(l)}$

- **Example:**  $\mathbf{h}_v^{(l)} = \text{Concat} \left( \text{Sum} \left( \left\{ \mathbf{m}_u^{(l)}, u \in N_r(v) \right\} \right) \right)$

# Recap: Layer connectivity

- **(3) Layer connectivity**
  - Add skip connections, pre/post-process layers



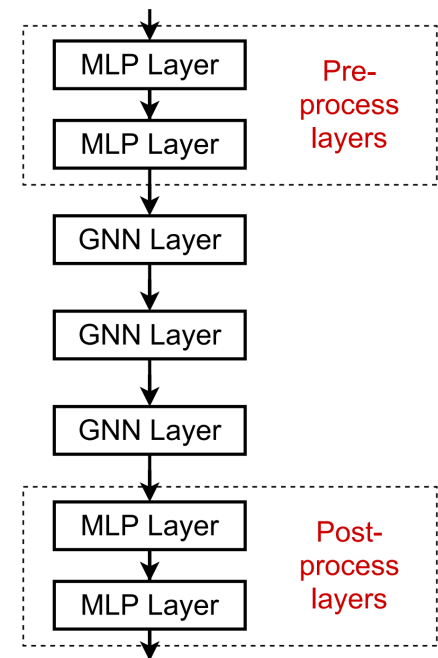
**Pre-processing layers:** Important when encoding node features is necessary.  
E.g., when nodes represent images/text

**Post-processing layers:** Important when reasoning / transformation over node embeddings are needed  
E.g., graph classification, knowledge graphs

**In practice, adding these layers works great!**

# Heterogeneous GNN Layers

- **Heterogeneous pre/post-process layers:**
  - MLP layers **with respect to each node type**
    - Since the output of GNN are **node embeddings**
  - $\mathbf{h}_v^{(l)} = \text{MLP}_{T(v)}(\mathbf{h}_v^{(l)})$ 
    - $T(v)$  is the type of node  $v$
- Other successful GNN designs are also encouraged for heterogeneous GNNs: skip connections, batch/layer normalization, ...



# Recap: Graph Manipulation

- **Graph Feature manipulation**
  - The input graph **lacks features** → **feature augmentation**
- **Graph Structure manipulation**
  - The graph is **too sparse** → **Add virtual nodes / edges**
  - The graph is **too dense** → **Sample neighbors when doing message passing**
  - The graph is **too large** → **Sample subgraphs to compute embeddings**
    - Will cover later in lecture: Scaling up GNNs

# Heterogeneous Graph Manipulation

- **Graph Feature manipulation**
  - **2 Common options:** compute graph statistics (e.g., node degree) within each relation type, or across the full graph (ignoring the relation types)
- **Graph Structure manipulation**
  - Neighbor and subgraph sampling are also common for heterogeneous graphs.
  - **2 Common options:** sampling within each relation type (ensure neighbors from each type are covered), or sample across the full graph

# Recap: GNN Prediction Heads

## Node-level prediction:

- $\hat{\mathbf{y}}_v = \text{Head}_{\text{node}}(\mathbf{h}_v^{(L)}) = \mathbf{W}^{(H)} \mathbf{h}_v^{(L)}$

## Edge-level prediction:

- $\hat{\mathbf{y}}_{uv} = \text{Head}_{\text{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}) =$   
 $\text{Linear}(\text{Concat}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}))$

## Graph-level prediction:

- $\hat{\mathbf{y}}_G = \text{Head}_{\text{graph}}(\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\})$

# Heterogeneous Prediction Heads

## Node-level prediction:

- $\hat{\mathbf{y}}_v = \text{Head}_{\text{node}, T(v)}(\mathbf{h}_v^{(L)}) = \mathbf{W}_{T(v)}^{(H)} \mathbf{h}_v^{(L)}$

## Edge-level prediction:

- $\hat{\mathbf{y}}_{uv} = \text{Head}_{\text{edge}, r}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}) =$   
 $\text{Linear}_r(\text{Concat}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}))$

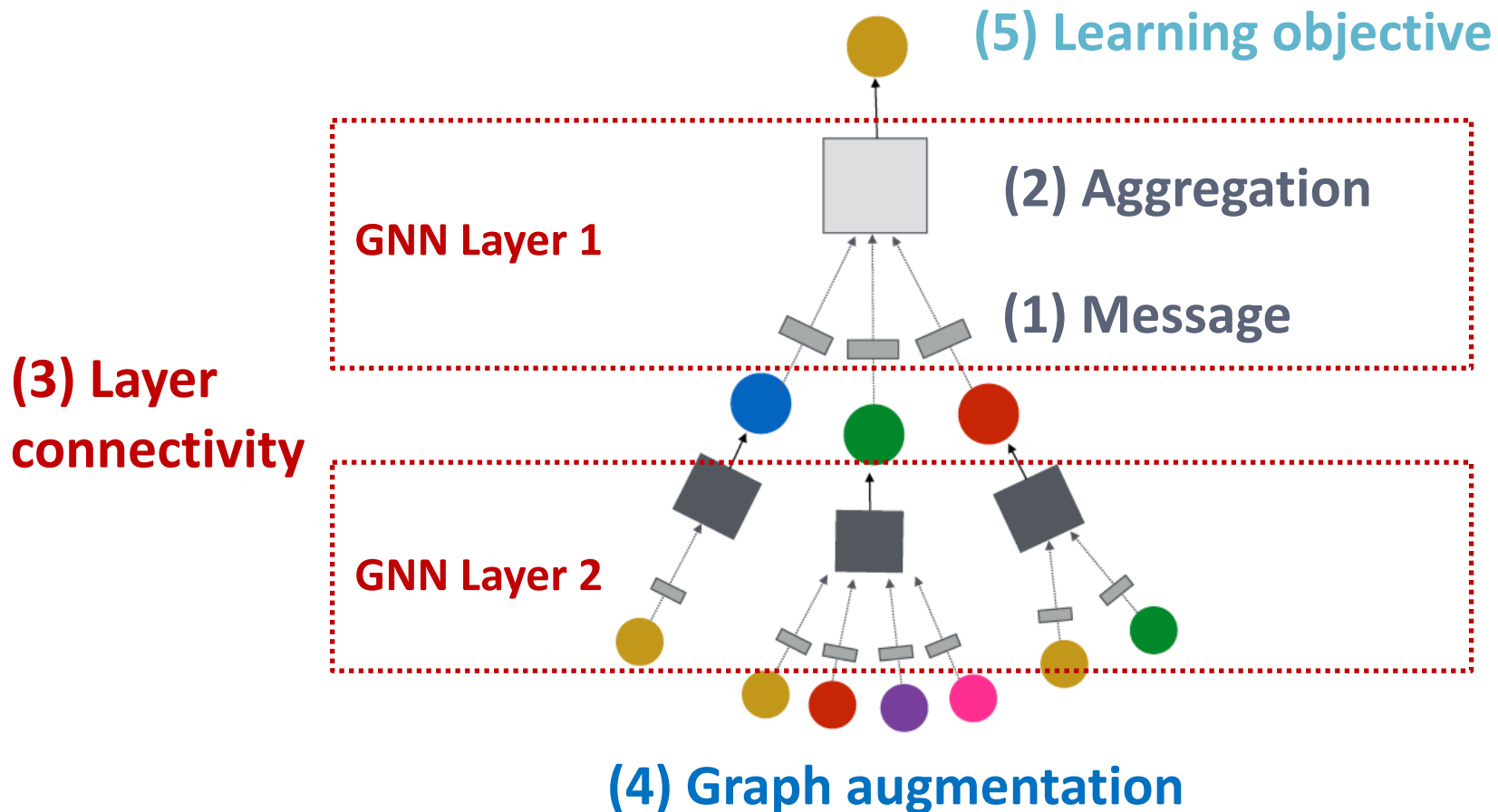
## Graph-level prediction:

- $\hat{\mathbf{y}}_G = \text{AGG}(\text{Head}_{\text{graph}, i}(\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall T(v) = i\}))$



# Summary: Heterogeneous GNN

Heterogeneous GNNs extend GNNs by separately modeling node/relation types + additional AGG



# Summary of the Lecture

- **Heterogeneous graphs:** graphs with multiple nodes or edge types
  - **Key concept: relation type** (node\_s, edge, node\_e)
  - Be aware that we don't always need heterogeneous graphs
- Learning with **heterogeneous graphs**
  - **Key idea:** separately model each relation type
  - **Relational GCNs**
  - Heterogeneous Graph Transformer
  - **Design space for heterogeneous GNNs**