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Stanford CS224W: Machine Learning with Heterogeneous Graphs

CS224W: Machine Learning with Graphs
Charilaos Kanatsoulis and Jure Leskovec, Stanford
University

<http://cs224w.stanford.edu>



Announcements

- **Project Proposal** due **today**
 - Gradescope submissions close at 11:59 PM
 - We are working on obtaining Google Cloud compute credits – updates to come
 - Project rubrics for each type are on course website
- **Colab 2** due this Thursday 10/23
- **Homework 2** out now, due Thursday 10/30

Response to high-resolution feedback

- **QueueStatus during OH**
 - We will ensure that all CAs use it for consistency
- **Practice midterm**
 - We will provide practice questions closer to the exam date

Stanford CS224W: Heterogeneous Graphs

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

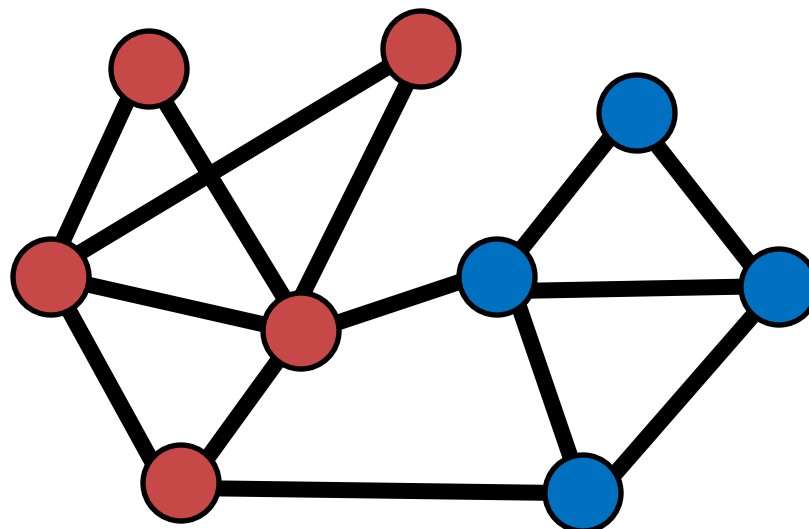
<http://cs224w.stanford.edu>



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
 - Design space for heterogeneous GNNs
 - Heterogeneous Graph Transformer (**Time permitting**)

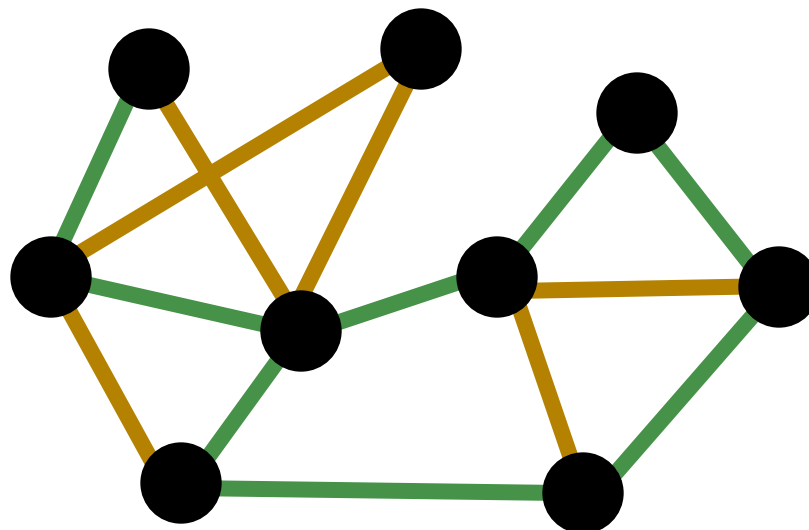
Heterogeneous Graphs: Motivation



2 types of nodes:

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

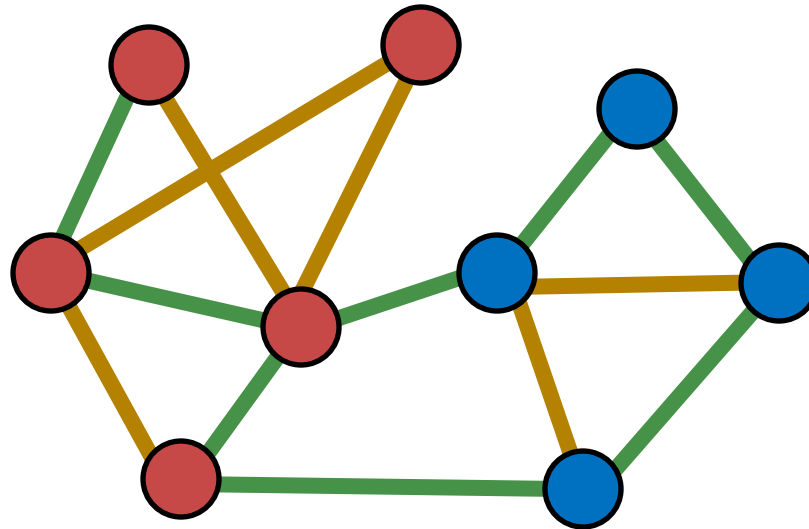
Heterogeneous Graphs: Motivation



2 types of edges:

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

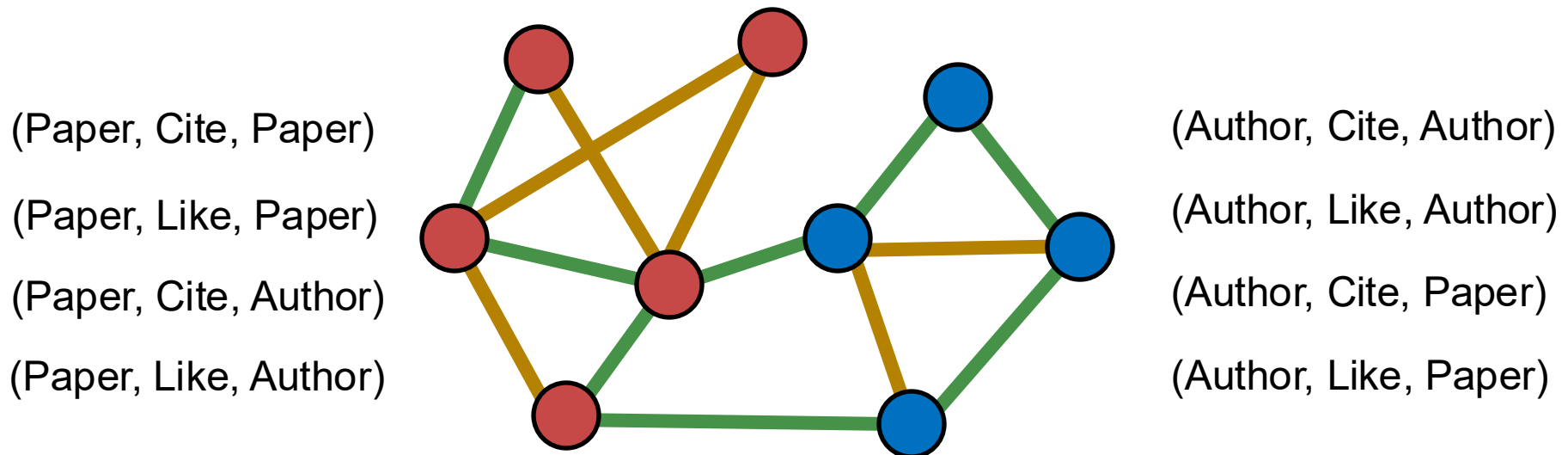
Heterogeneous Graphs: Motivation



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 $(u, v) \in E$

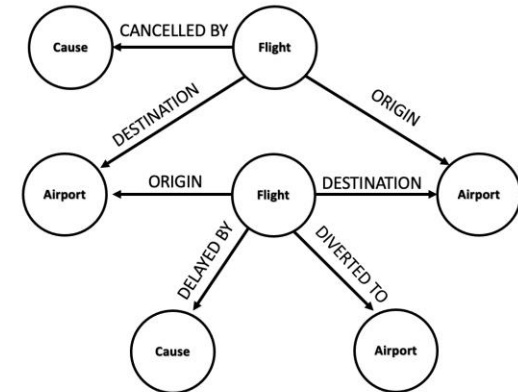
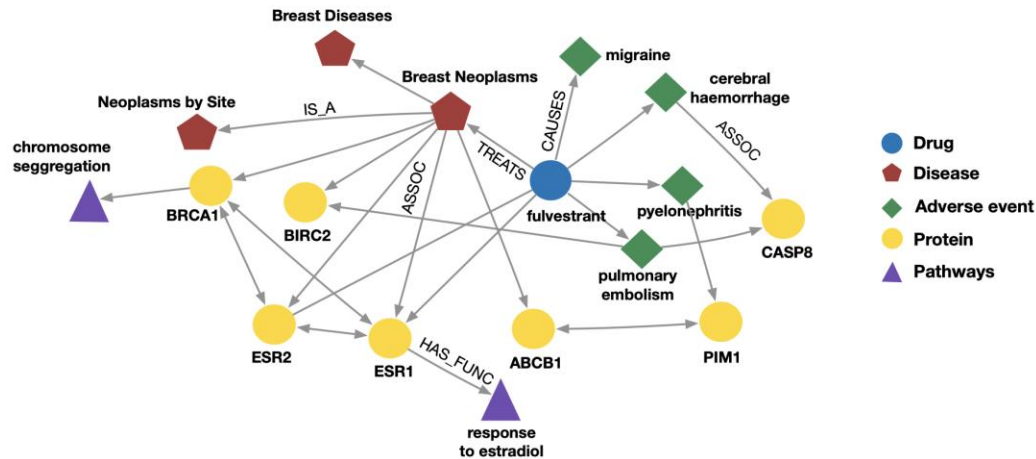
- **Edge type** for edge (u, v) : $\phi(u, v)$

- **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

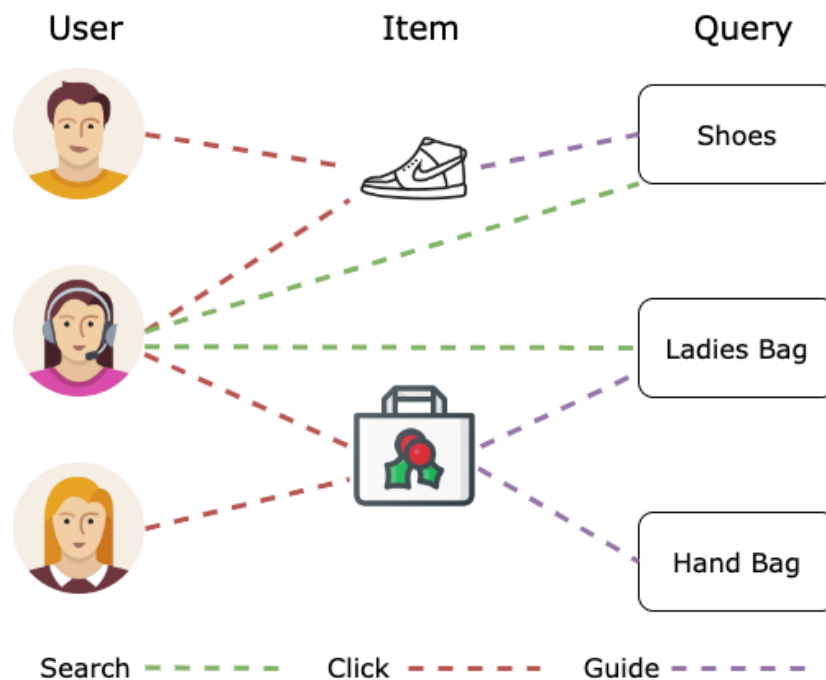
Example relation: (UA689, Origin, LAX)

Example node type: Flight

Example edge type: Destination

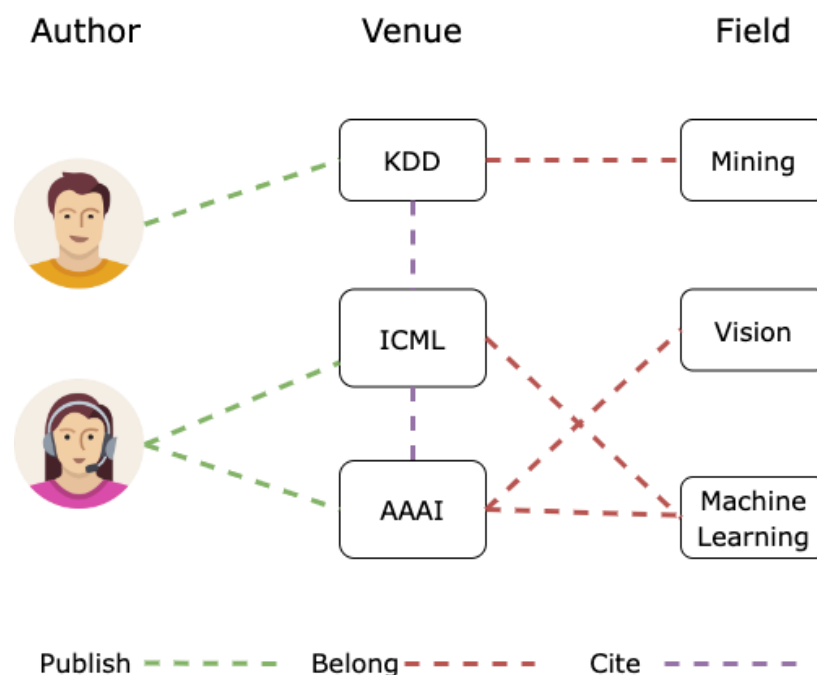
Many Graphs are Heterogeneous Graphs (2)

- 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
- There are many ways to **convert a heterogeneous graph to a standard graph** (that is, a homogeneous graph)

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

Stanford CS224W: Relational GCN (RGCN)

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



Recap: Classical GNN Layers: GCN

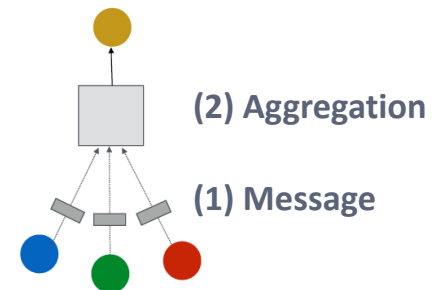
■ (1) Graph Convolutional Networks (GCN)

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

■ How to write this as Message + Aggregation?

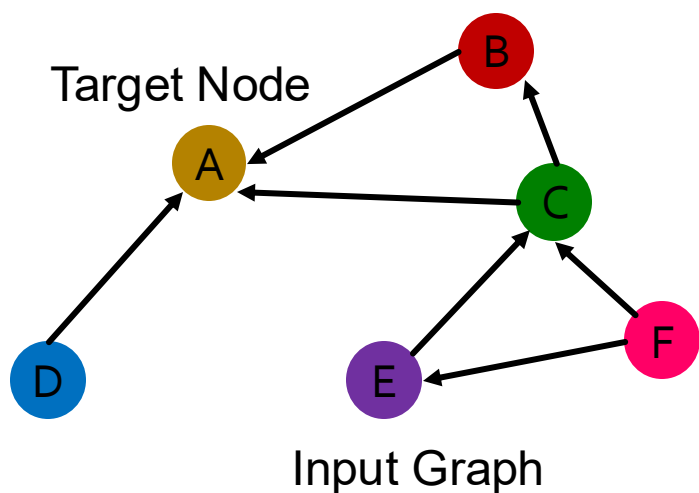
$$\mathbf{h}_v^{(l)} = \sigma \left(\underbrace{\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}}_{\text{Aggregation}} \right)$$

Message



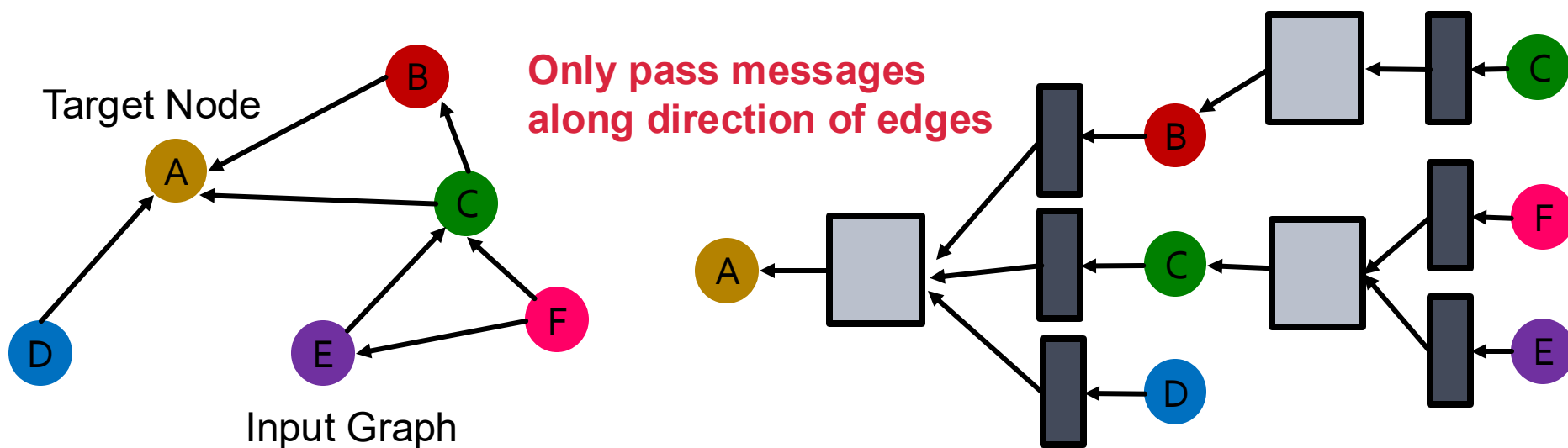
Relational GCN

- 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?



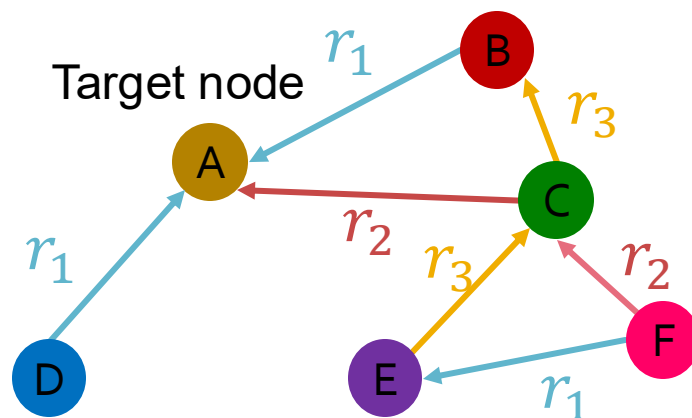
Relational GCN

- We will extend **GCN** to handle heterogeneous graphs with multiple edge/relation types
- We start with a **directed graph** with **one** relation
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Relational GCN (1)

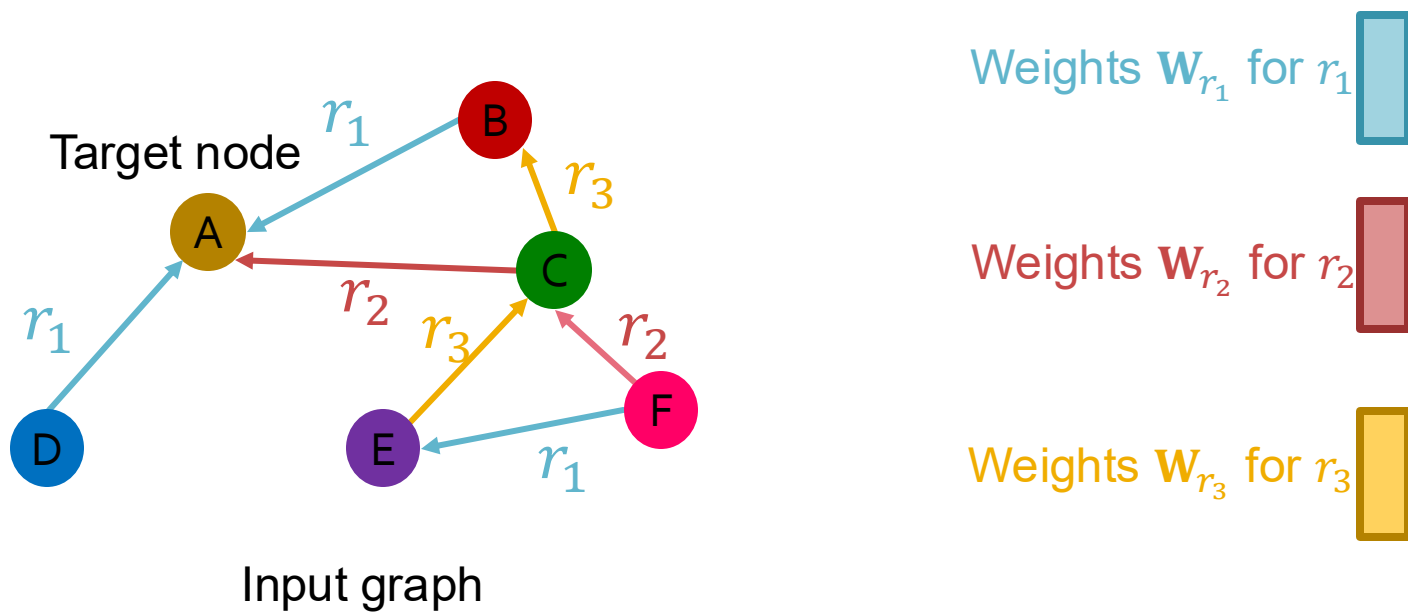
- What if the graph has **multiple relation types**?



Input graph

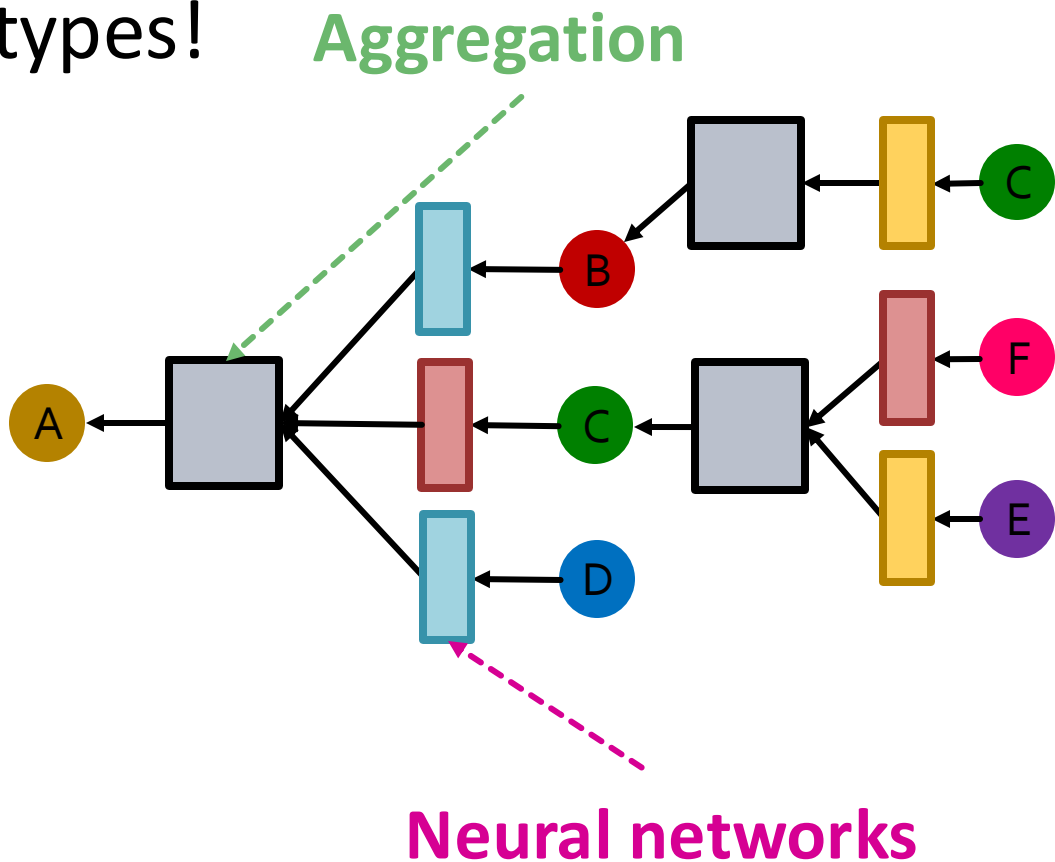
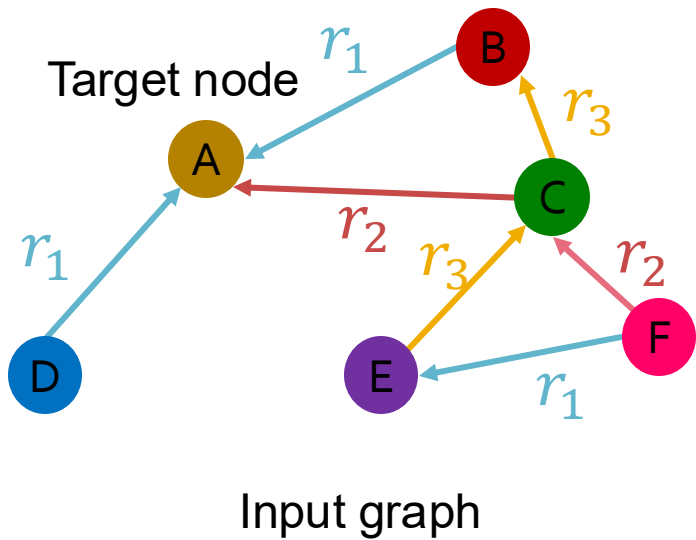
Relational GCN (2)

- 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! **Aggregation**



Recap: Classical GNN Layers: GCN

■ (1) Graph Convolutional Networks (GCN)

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

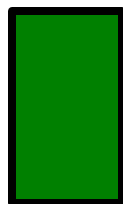
■ We add a self-loop

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

Relational GCN (4)

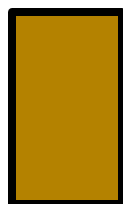
- Introduce a set of neural networks for each relation type!

Weight for rel_1

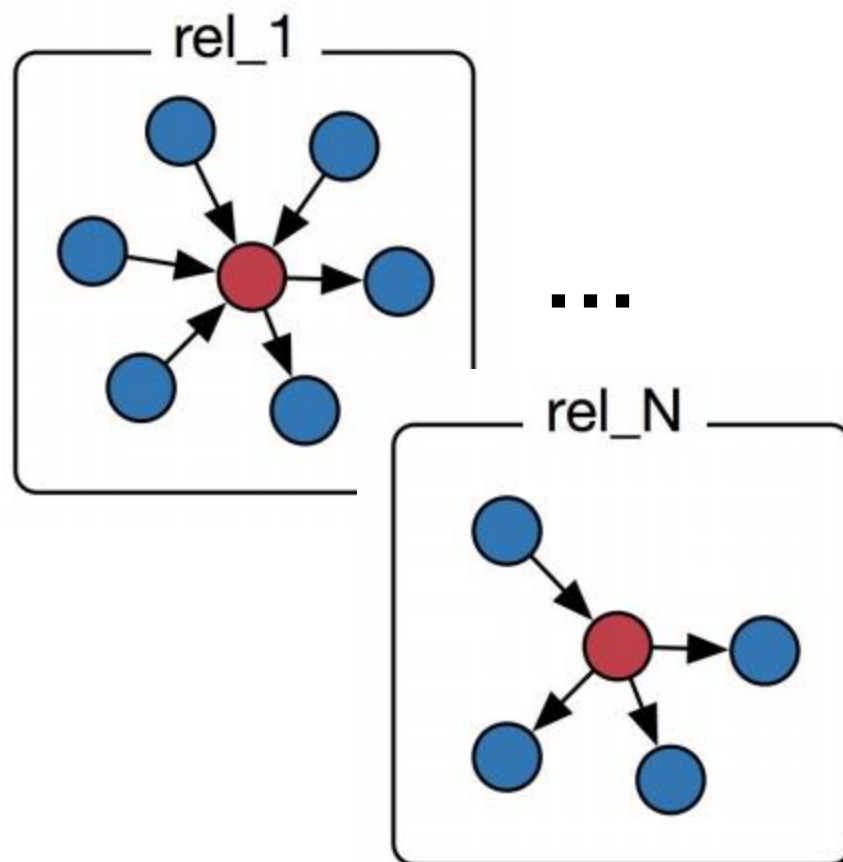
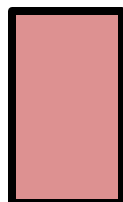


...

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

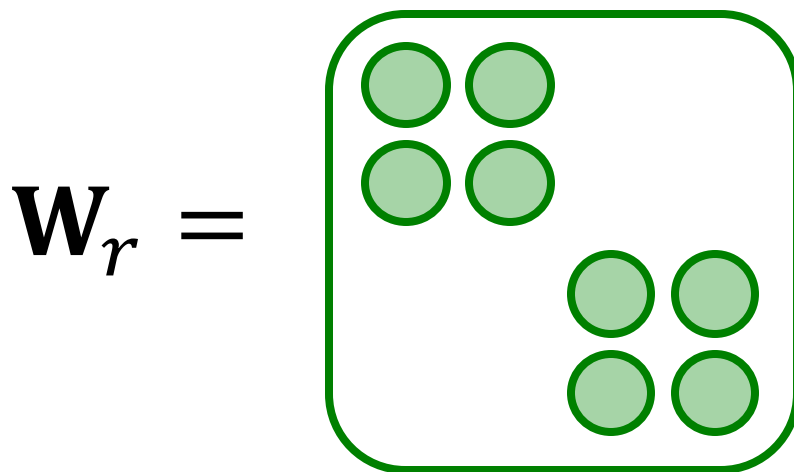
- $\mathbf{h}_v^{(l+1)} = \sigma \left(\text{Sum} \left(\left\{ \mathbf{m}_{u,r}^{(l)}, u \in N(v) \right\} \cup \left\{ \mathbf{m}_v^{(l)} \right\} \right) \right)$

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 blocks, then # param reduces from

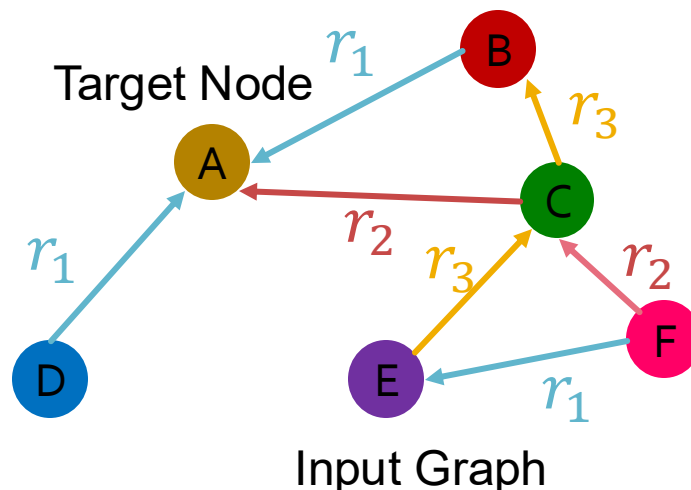
$$d^{(l+1)} \times d^{(l)} \text{ to } B \times \frac{d^{(l+1)}}{B} \times \frac{d^{(l)}}{B}$$

(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

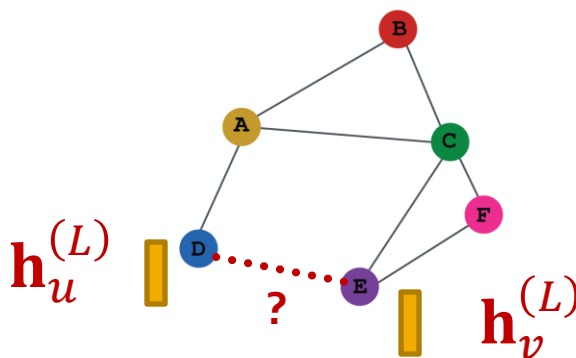
Example: Entity/Node Classification

- **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:** Make prediction using pairs of node embeddings
- $\hat{y}_{uv} = f(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$



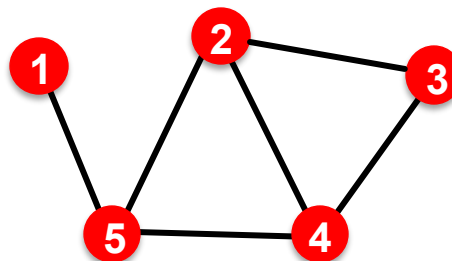
- What are the options for $f(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$?

Prediction Heads: Link Prediction

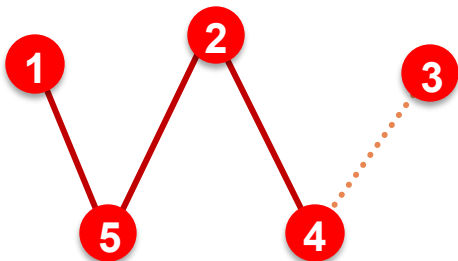
- Options for $f(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$:
- **Dot product**
 - $\hat{y}_{uv} = (\mathbf{h}_u^{(L)})^T \mathbf{h}_v^{(L)}$
 - This approach only applies to 1-way prediction (e.g., link prediction: predict the existence of an edge)

Setting up Link Prediction

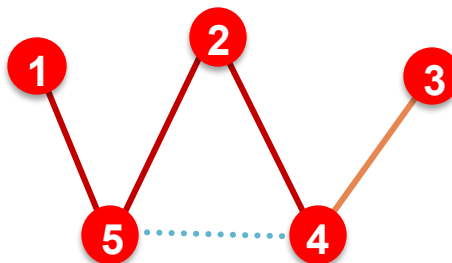
■ Transductive link prediction split:



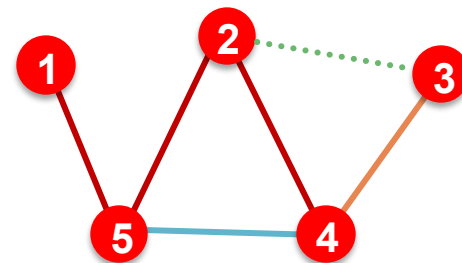
The original graph



(1) At training time:
Use **training message edges** to predict **training supervision edges**



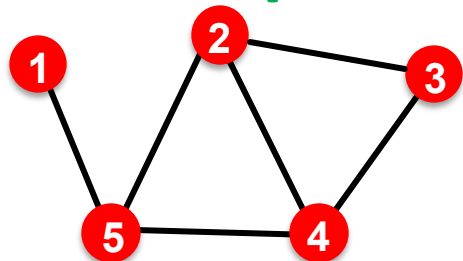
(2) At validation time:
Use **training message edges & training supervision edges** to predict **validation edges**



(3) At test time:
Use **training message edges & training supervision edges & validation edges** to predict **test edges**

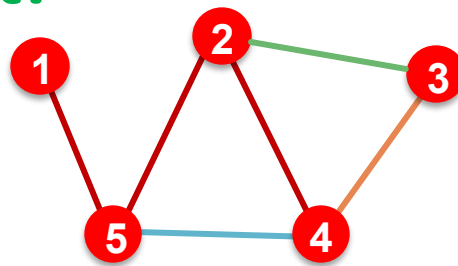
Example: Link Prediction

■ Link prediction split:



The original graph

Split
→



Split Graph with 4 categories of edges

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

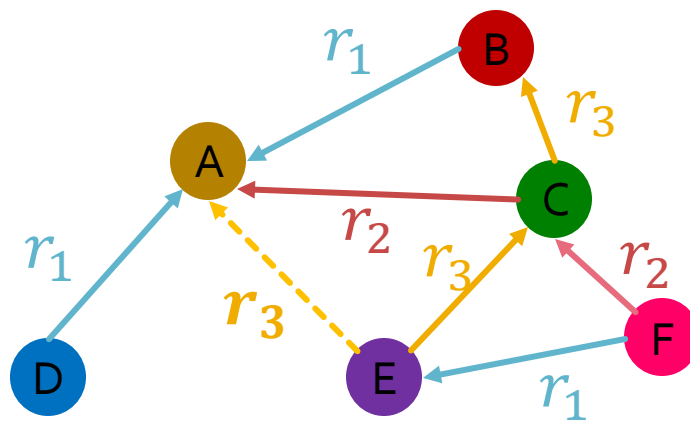
Training message edges
Training supervision edges
Validation edges
Test edges

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.

RGCN for Link Prediction (1)

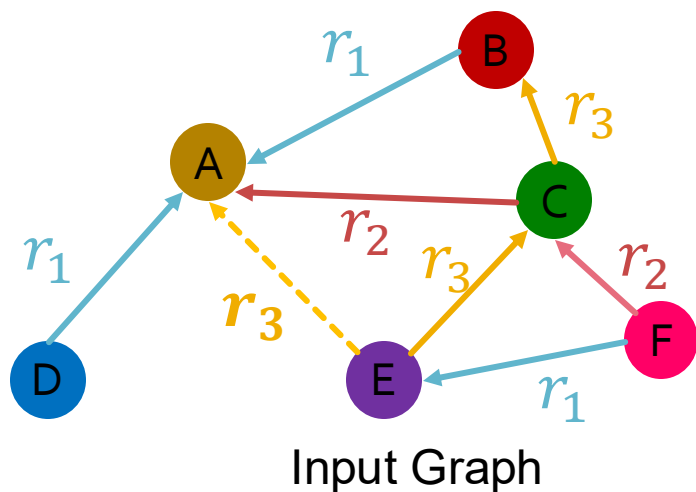
- Assume (E, r_3, A) is training supervision edge, all the other edges are training message edges
- Use RGCN to score (E, r_3, A) !
 - Take the final layer of E and A : $\mathbf{h}_E^{(L)}$ and $\mathbf{h}_A^{(L)} \in \mathbb{R}^d$
 - Relation-specific score function $f_r: \mathbb{R}^d \times \mathbb{R}^d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



Input Graph

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)

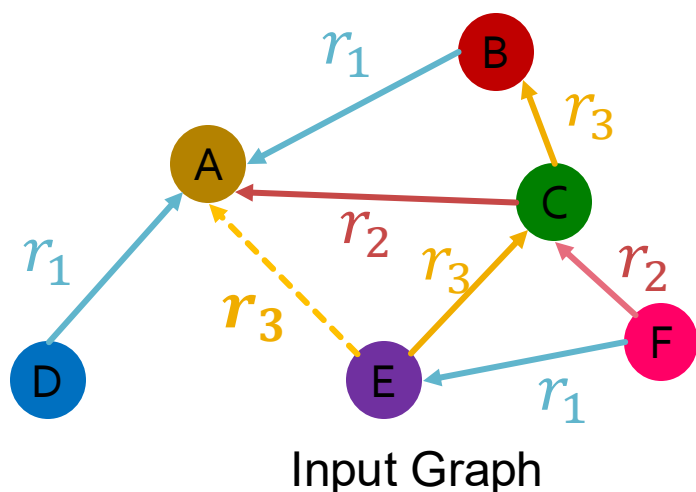
training supervision edges: (E, r_3, A)
training message edges: all the rest existing edges (solid lines)

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**

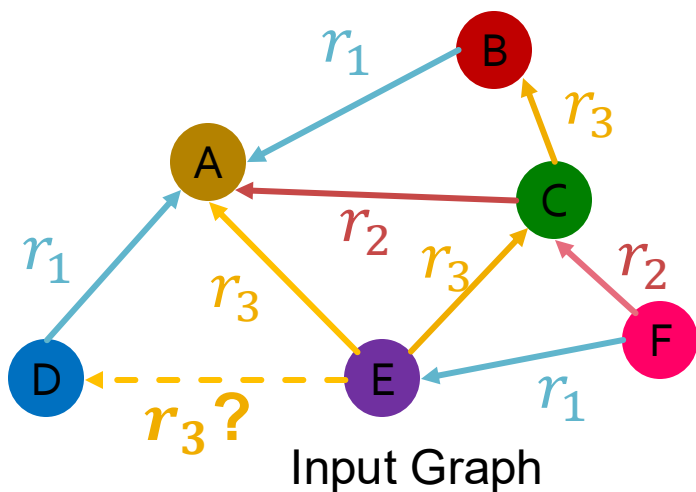
$$\ell = -\log \sigma \left(f_{r_3}(h_E, h_A) \right) - \log(1 - \sigma(f_{r_3}(h_E, h_B)))$$

σ ... 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)

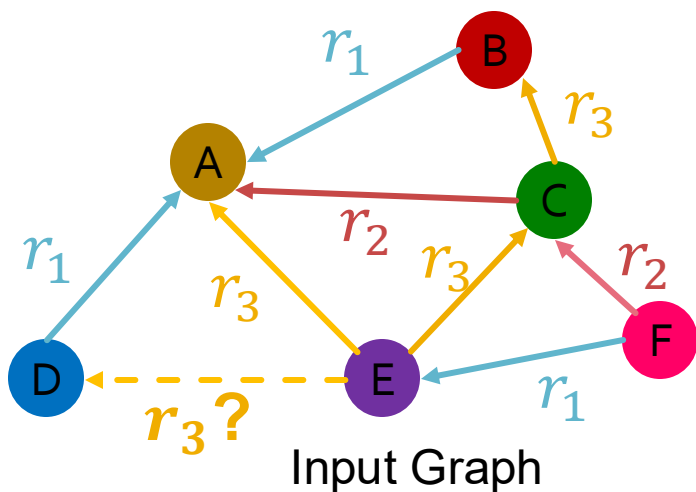
(2) At validation time:

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)

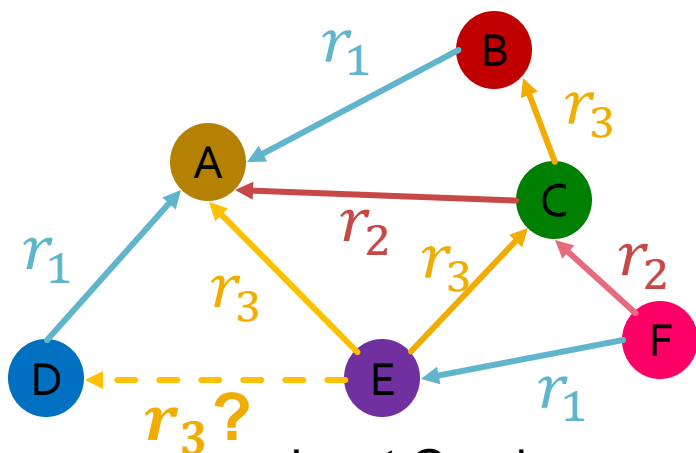
Intuition: the score of (E, r_3, D) should be higher than all (E, r_3, v) where (E, r_3, v) is **NOT** in the **training message edges** and **training supervision edges**, e.g., (E, r_3, B)

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

RGCN for Link Prediction (6)

■ Evaluation:

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



Input Graph

$$f_{r_3}(E, r_3, D)$$

$$f_{r_3}(E, r_3, B)$$

$$f_{r_3}(E, r_3, F)$$

RK of (E, r_3, D) : 1

1. Hits@2 = 1

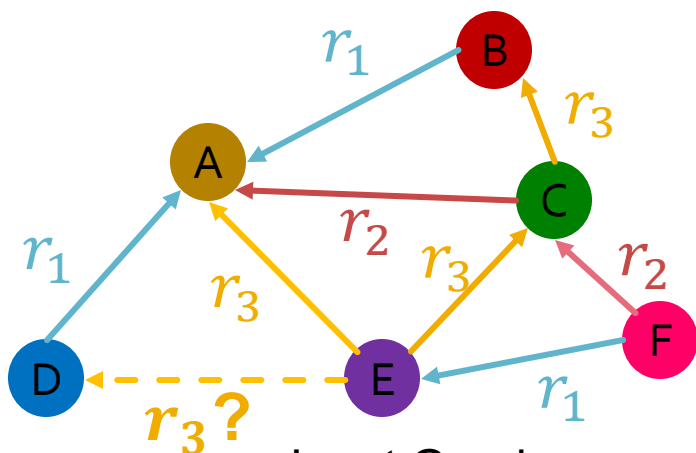
2. Reciprocal Rank: $\frac{1}{1}$

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**
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RGCN for Link Prediction (6)

■ Evaluation:

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



Input Graph

$$f_{r_3}(E, r_3, B)$$

$$f_{r_3}(E, r_3, D)$$

$$f_{r_3}(E, r_3, F)$$

RK of (E, r_3, D) : 2

1. Hits@2 = 1

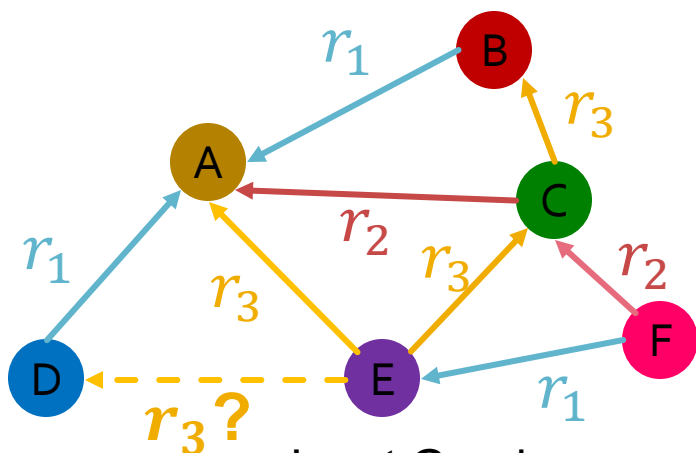
2. Reciprocal Rank: $\frac{1}{2}$

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

RGCN for Link Prediction (6)

■ Evaluation:

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



Input Graph

$$f_{r_3}(E, r_3, B)$$

$$f_{r_3}(E, r_3, F)$$

$$f_{r_3}(E, r_3, D)$$

RK of (E, r_3, D) : 3

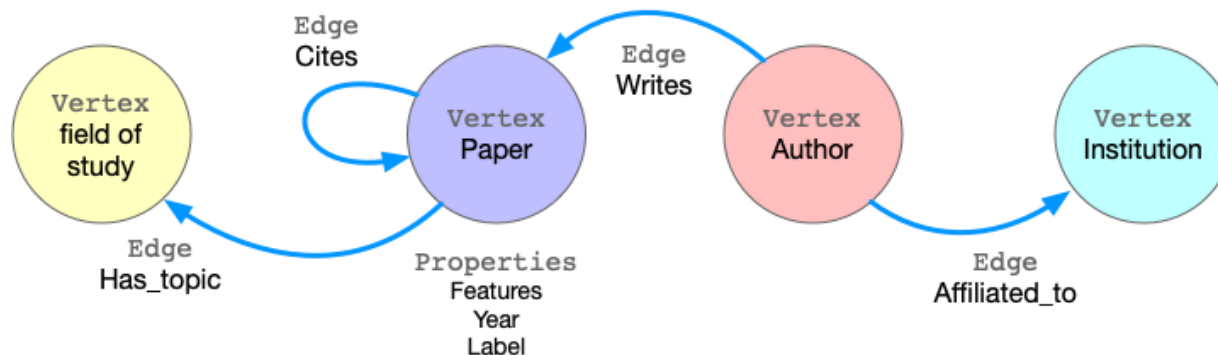
1. Hits@2 = 0

2. Reciprocal Rank: $\frac{1}{3}$

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**
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4. Calculate metrics
 1. Hits@ k : $1 [RK \leq k]$. Higher is better
 2. Reciprocal Rank: $\frac{1}{RK}$. Higher is better

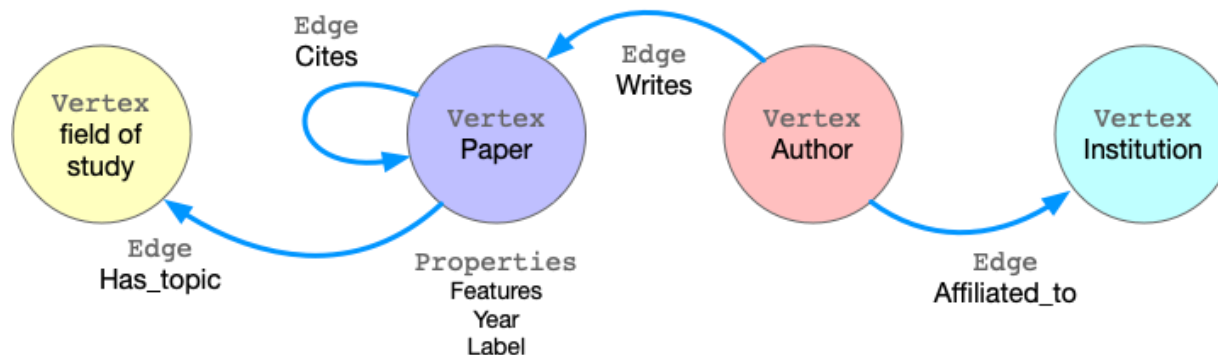
Benchmark for Heterogeneous Graphs (1)

- 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**



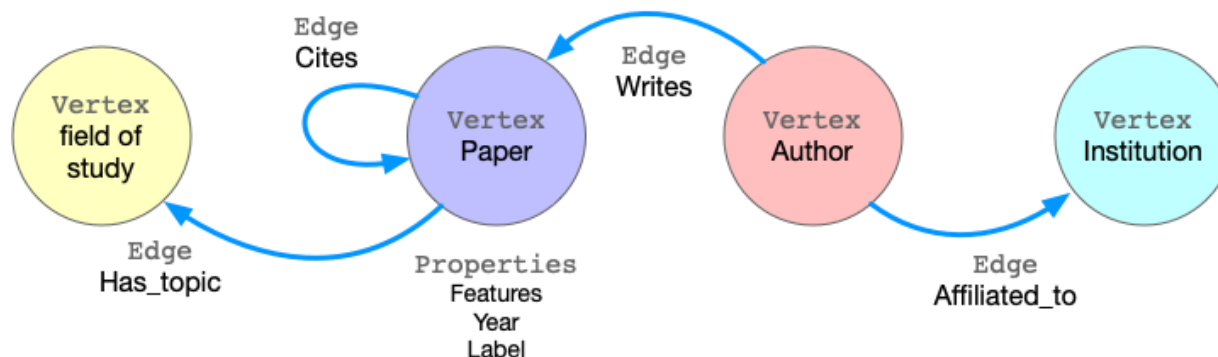
Benchmark for Heterogeneous Graphs (3)

■ 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:

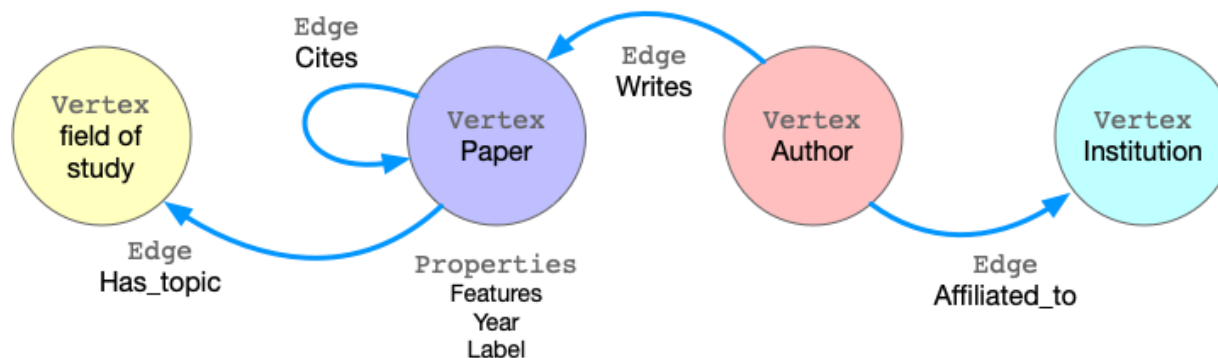
Rank	Method	Ext. data	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
1	SeHGNN (Complex embs)	No	0.5719 ± 0.0012	0.5917 ± 0.0009	Xiaocheng Yang (ICT-GIMLab)	Paper , Code	8,371,231	NVIDIA Tesla T4 (15 GB)	Jul 7, 2022
21	NeighborSampling (R-GCN aggr)	No	0.4678 ± 0.0067	0.4761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

SOTA

R-GCN

■ SOTA method: SeHGNN

- Complex (Next lecture) + Simplified GCN



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, RGIN, RGAT, etc.)
- **Benchmark:** **ogbn-mag** from Microsoft Academic Graph, to predict **paper venues**

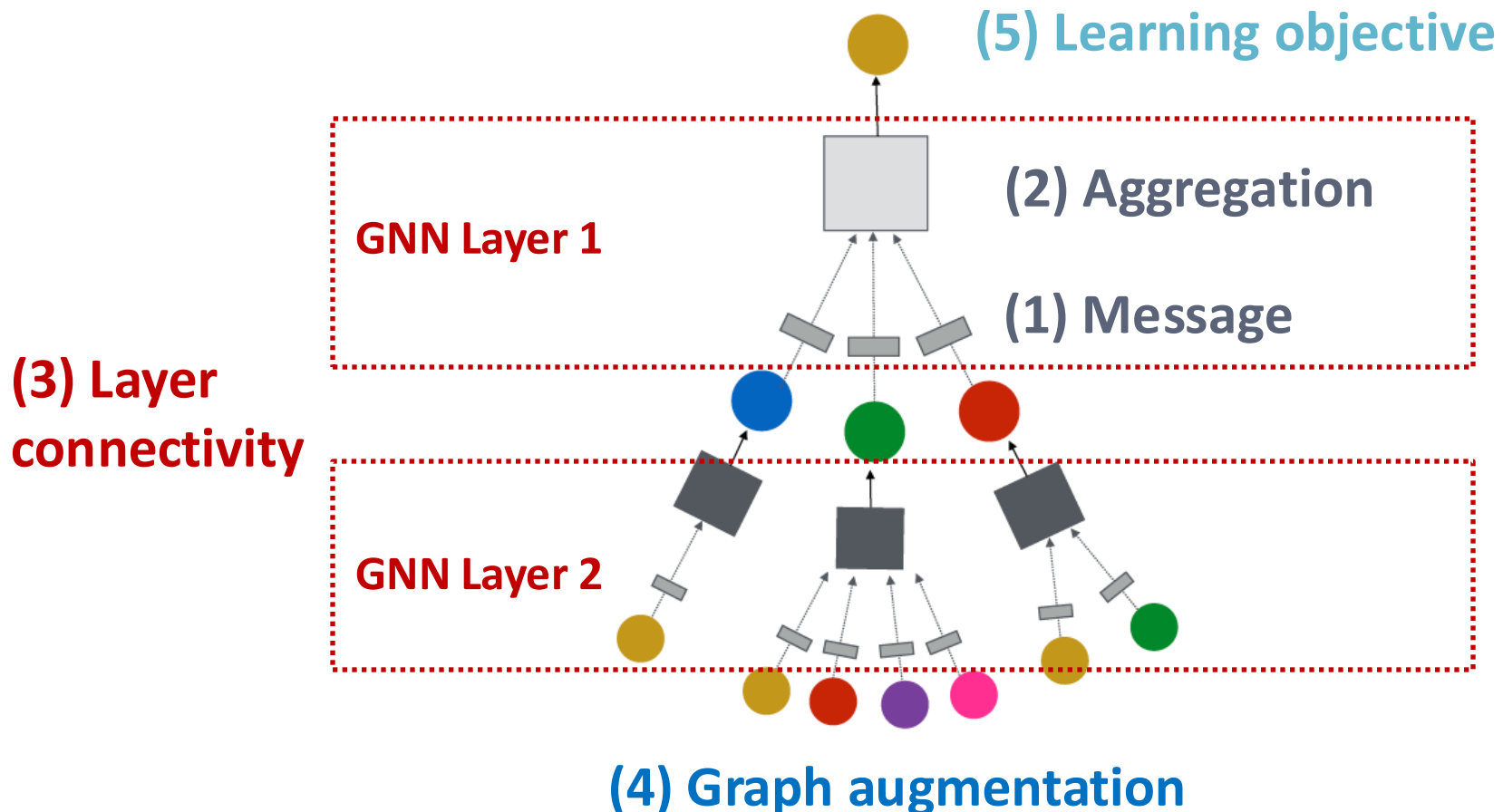
Stanford CS224W: Design Space of Heterogeneous GNNs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
<http://cs224w.stanford.edu>



Recap: GNN Framework

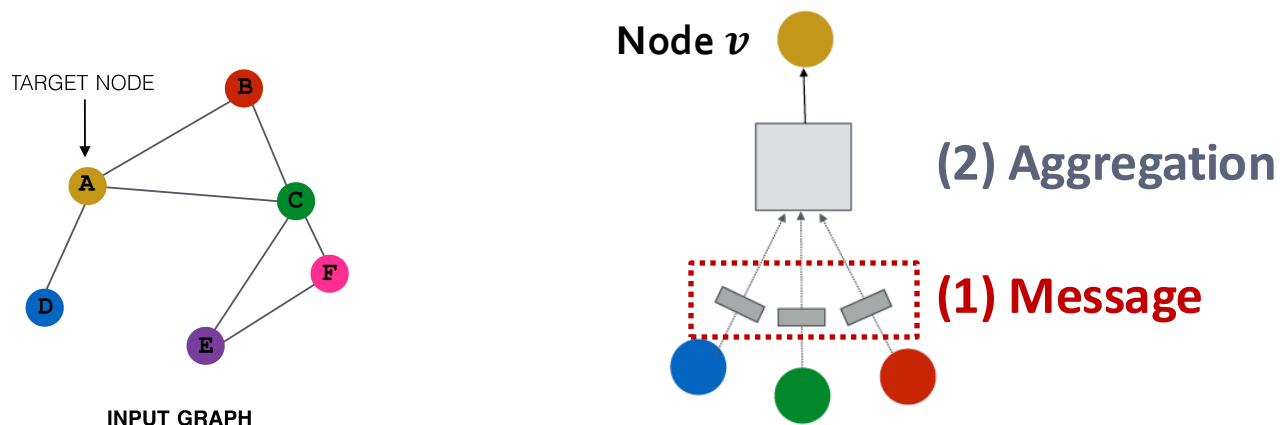
How do we extend the general GNN design space to heterogeneous graphs?



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

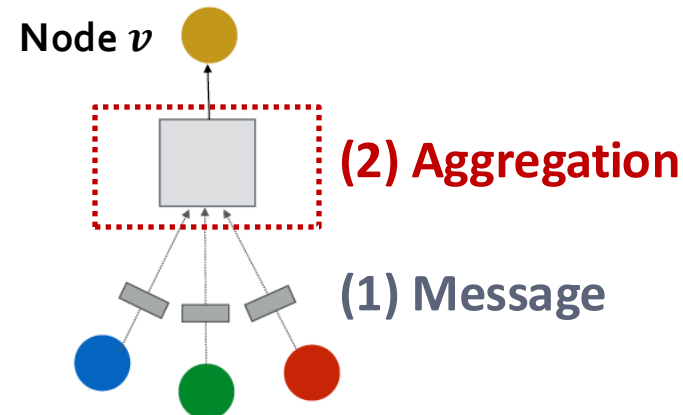
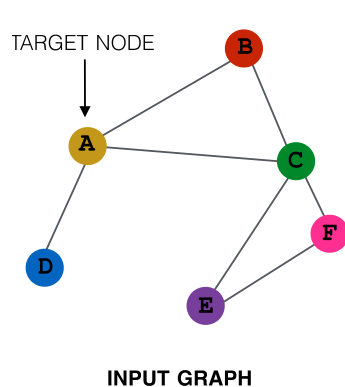
■ (2) Aggregation

- **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

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

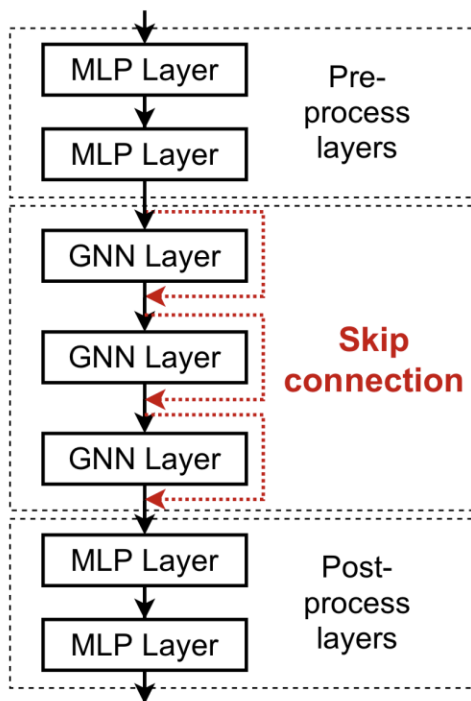
- Given all the messages sent to a node
- Within each message type, aggregate the messages that belongs to the relation type with $\text{AGG}_r^{(l)}$
- Aggregate across the edge types with $\text{AGG}_{all}^{(l)}$

- **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

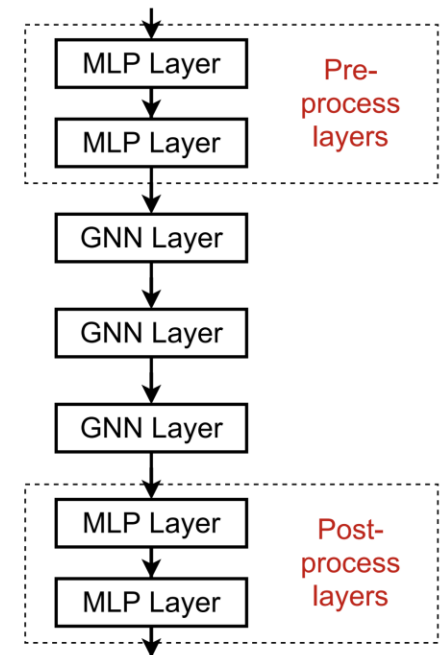
Post-processing layers: Important when reasoning / transformation over node embeddings are needed

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:

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

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** α_{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?**

Basics: Attention in Transformer

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

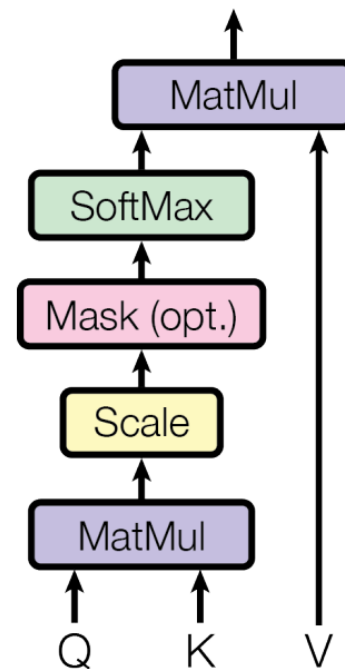
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

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
 - $Q = Q_Linear(X)$
 - $K = K_Linear(X)$
 - $V = V_Linear(X)$

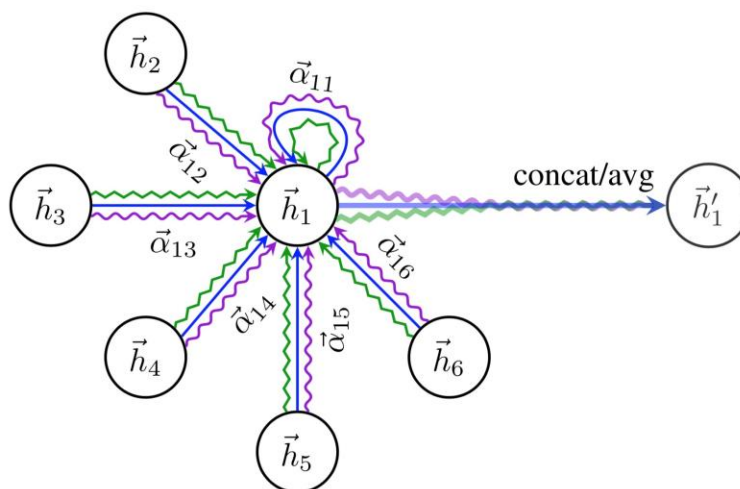


Heterogeneous Mutual Attention (1)

- **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?



From Transformers to GATs

- **Mutual Attention:**

$$ATT-head^i(s, t) = \left(K^i(s) Q^i(t)^T \right)$$

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

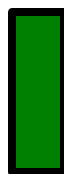
$$Q^i(t) = \text{Q-Linear}^i \left(H^{(l-1)}[t] \right)$$

- A set of neural networks for the attention scores of each edge.

Heterogeneous Graph Transformer

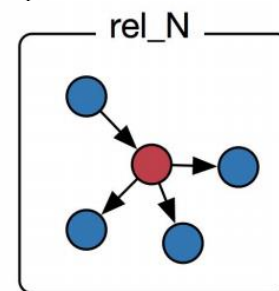
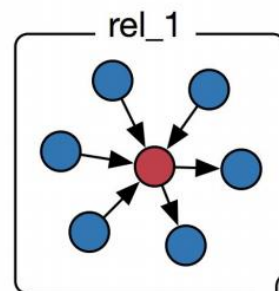
- **Motivation:** GAT is **unable to represent** different node & different edge types
- Introduce a set of neural networks for each relation type is **too expensive** for attention
 - **Recall:** relation describes (node_s, edge, node_e)

Weight for rel_1



...

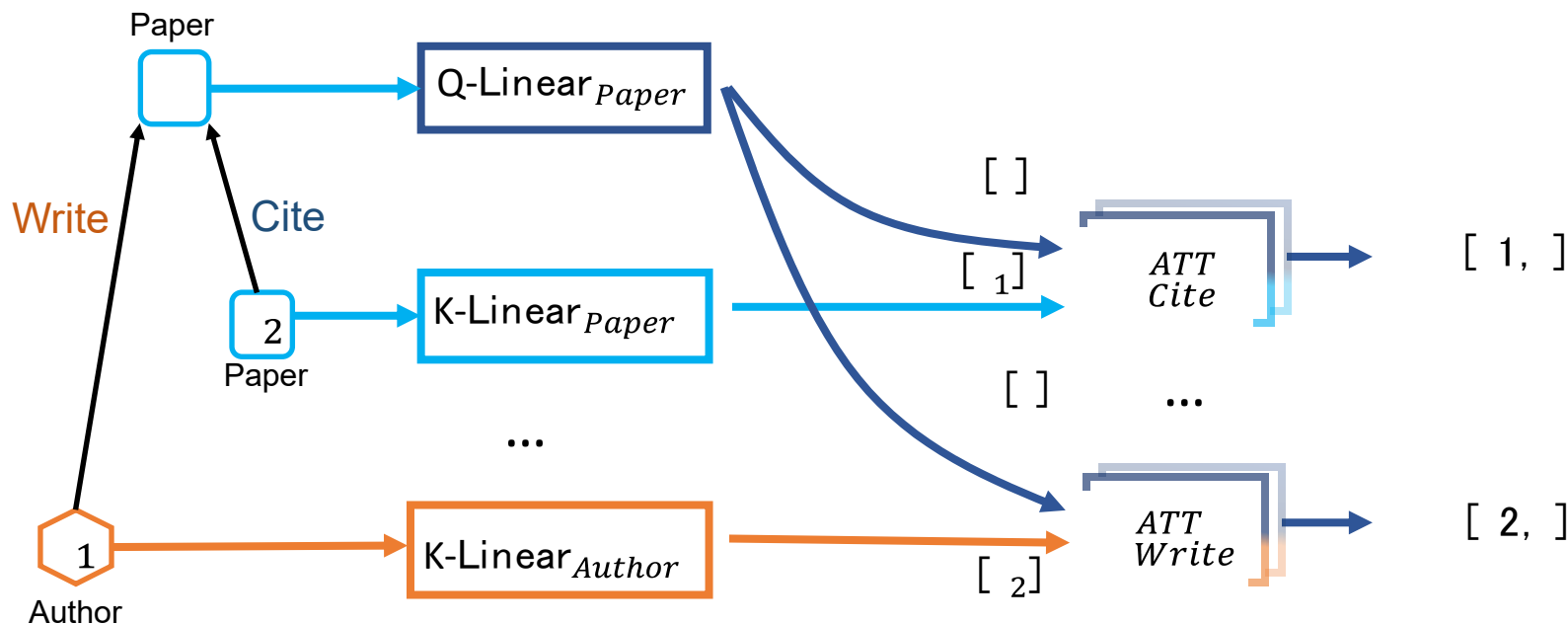
Weight for rel_N



Too expensive!

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

- **Heterogeneous Mutual Attention (First Attempt):**

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

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

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

- Introduce a set of neural networks for the attention scores of each relation type.
- **Too expensive** for attention!

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

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**

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

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

**Weights for
each node type**

**Weights for
each edge type**

HGT vs R-GCN: Performance

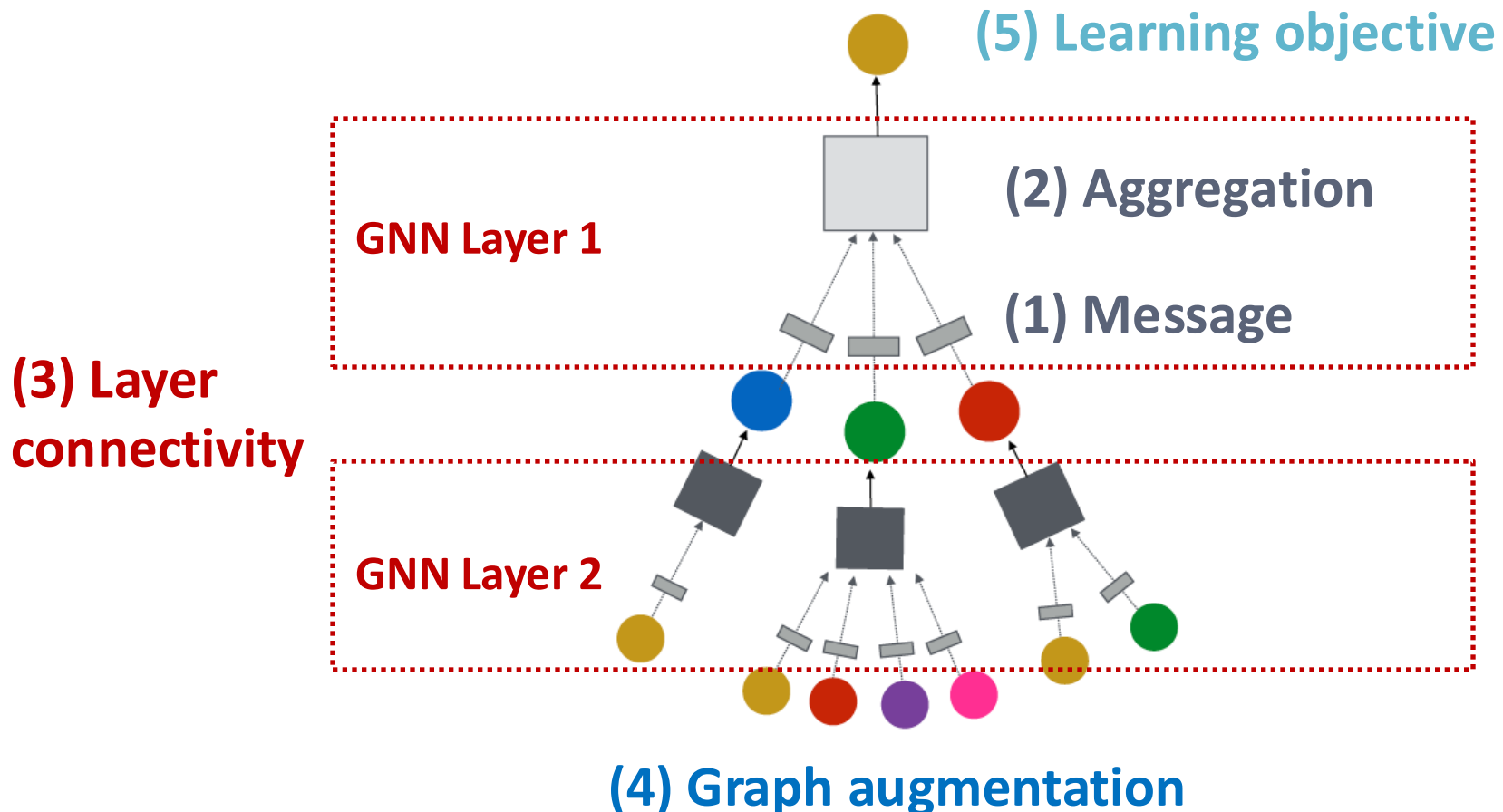
- **Benchmark:** [ogbn-mag](#) from Microsoft Academic Graph, to predict **paper venues**

Rank	Method	Ext. data	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
18	HGT (LADIES Sample)	No	0.4927 \pm 0.0061	0.4989 \pm 0.0047	Ziniu Hu	Paper , Code	21,173,389	Tesla K80 (12GB GPU)	Jan 26, 2021
21	NeighborSampling (R-GCN aggr)	No	0.4678 \pm 0.0067	0.4761 \pm 0.0068	Matthias Fey – OGB team	Paper , Code	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

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
 - Design space for heterogeneous GNNs
 - Heterogeneous Graph Transformer