Stanford CS224W: Machine Learning with Heterogeneous Graphs

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

ANNOUNCEMENTS

- **Project Proposal due today**

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**

Stanford CS224W: Heterogeneous Graphs

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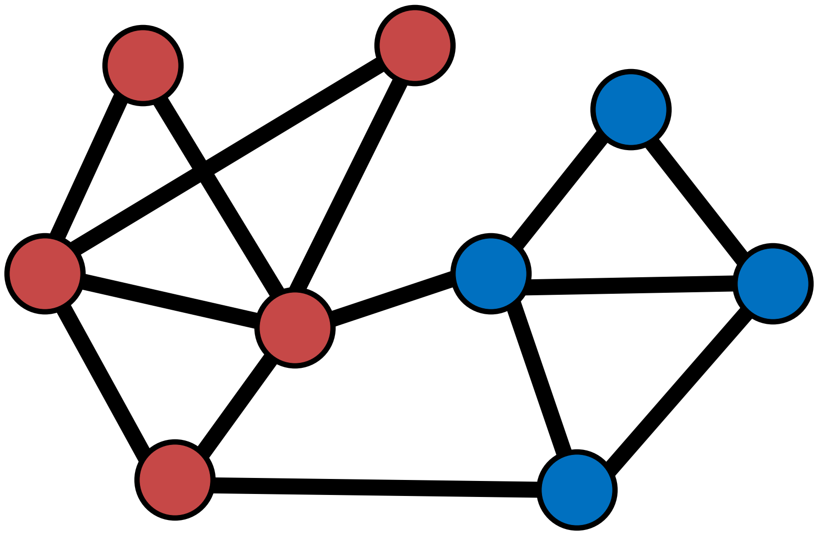
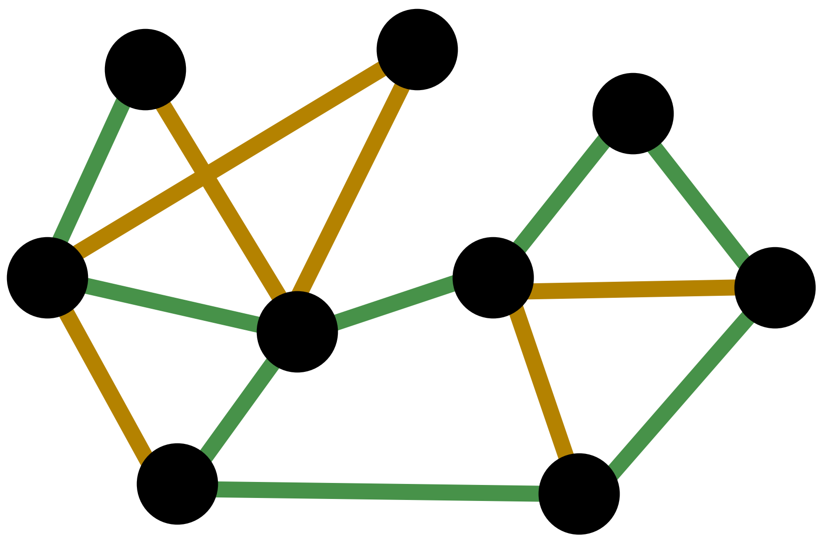
Heterogeneous Graphs: Motivation



2 types of nodes:

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

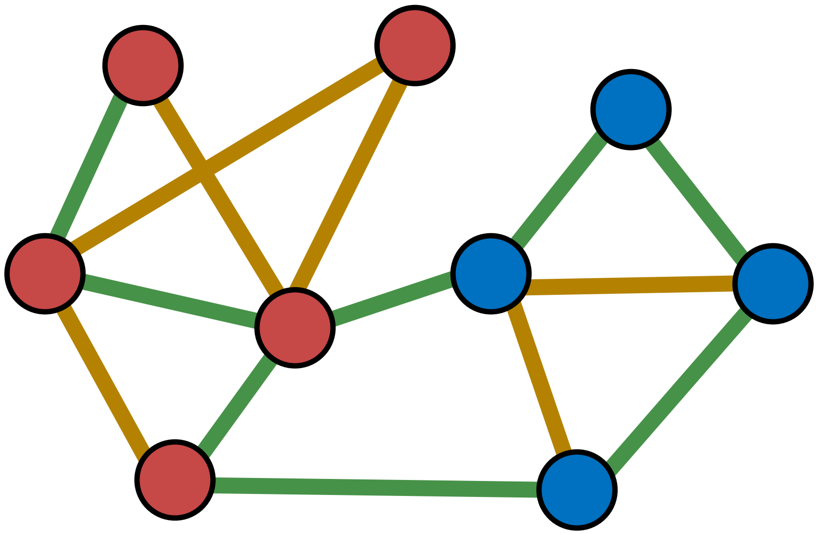
Heterogeneous Graphs: Motivation



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

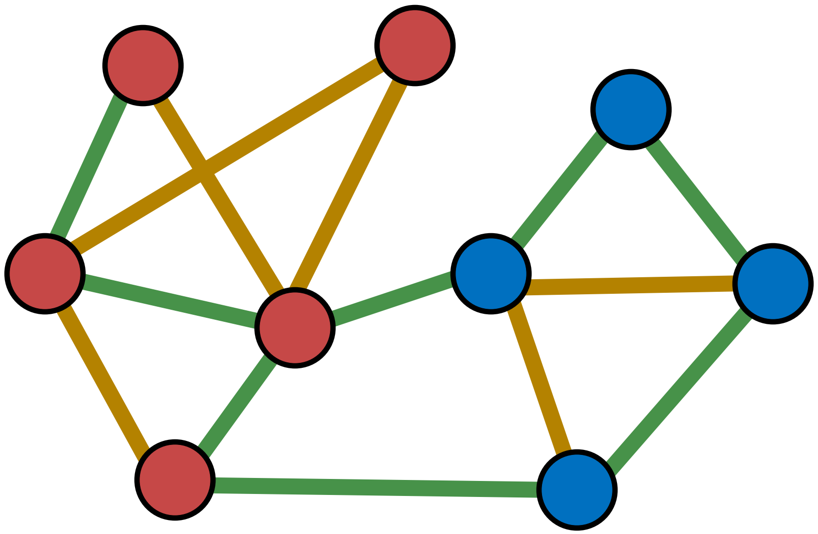
8 possible relation types!

(Paper, Cite, Paper)

(Paper, Like, Paper)

(Paper, Cite, Author)

(Paper, Like, Author)



(Author, Cite, Author)

(Author, Like, Author)

(Author, Cite, Paper)

(Author, Like, Paper)

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

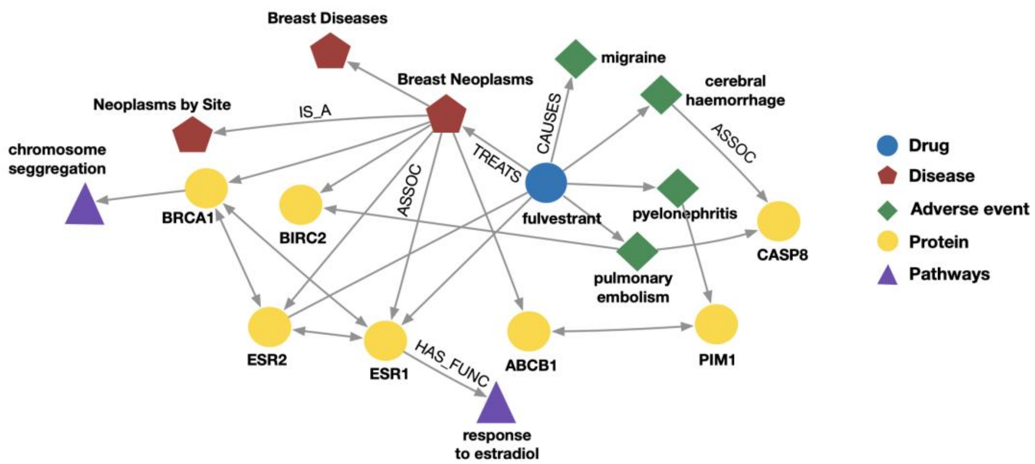
Heterogeneous Graphs

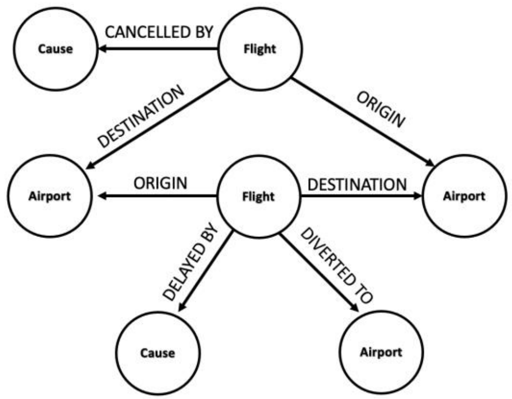
- **A heterogeneous graph is defined as**
$$\boldsymbol{G = (V, E, \tau, \phi)}$$
  - Nodes **with node types** $v \in V$
    - **Node type** for node v: $\tau(v)$
  - Edges **with edge types** $(u, v) \in E$
    - **Edge type** for edge (u, v): $\phi(u, v)$
    - **Relation type** for edge e is a tuple: $r(u, v) = (\tau(u), \phi(u, v), \tau(v))$

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

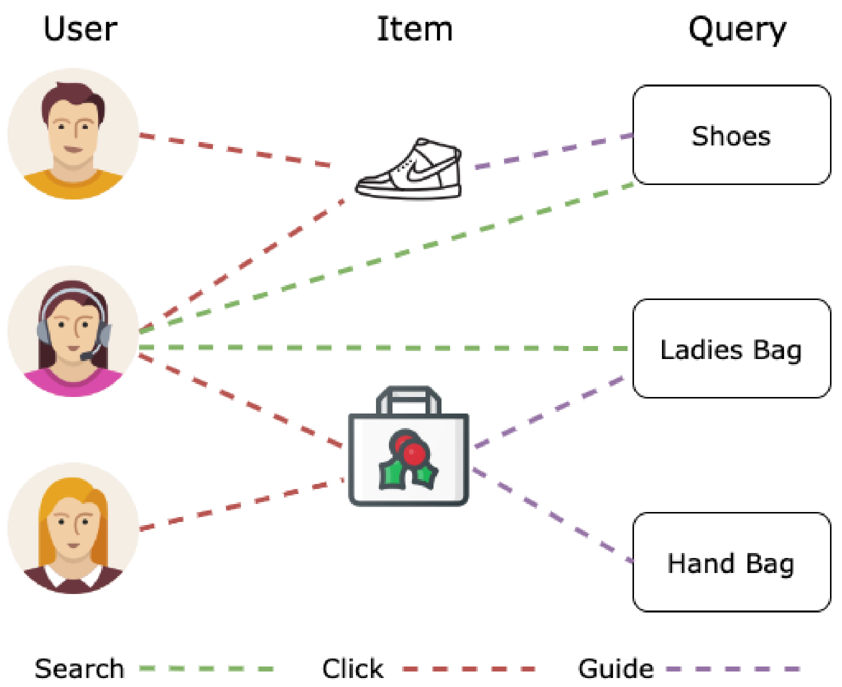
Example node: Migraine
Example relation: (fulvestrant, Treats, Breast Neoplasms)
Example node type: Protein
Example edge type: Causes

Event Graphs

Example node: SFO
Example relation: (UA689, Origin, LAX)
Example node type: Flight
Example edge type: Destination

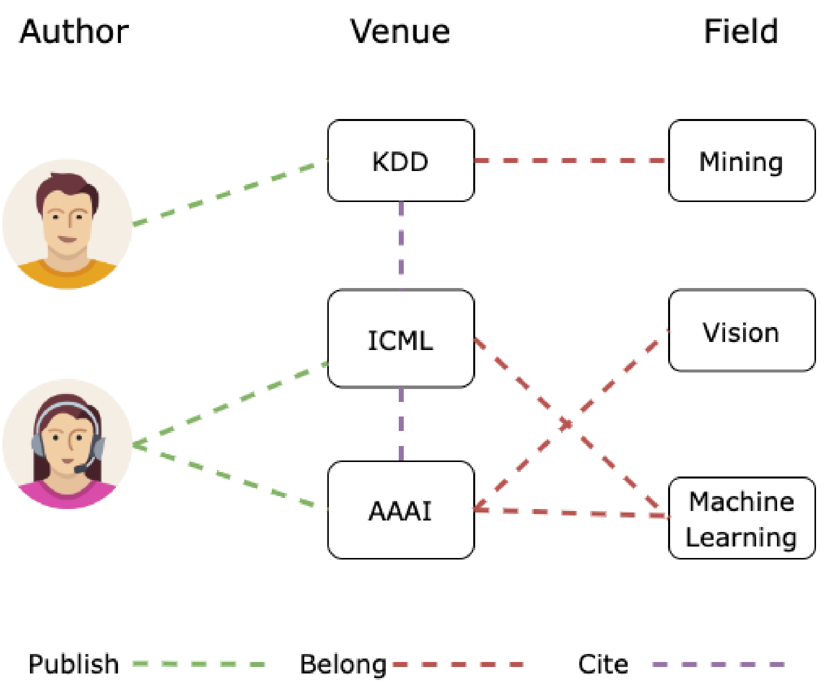
Many Graphs are Heterogeneous Graphs (2)

- 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
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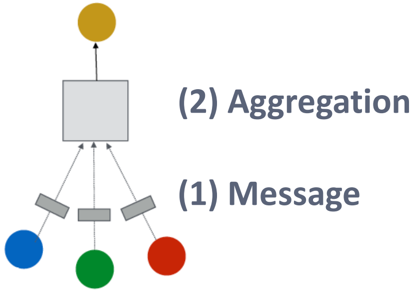
Recap: Classical GNN Layers: GCN

- **(1) Graph Convolutional Networks (GCN)**

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

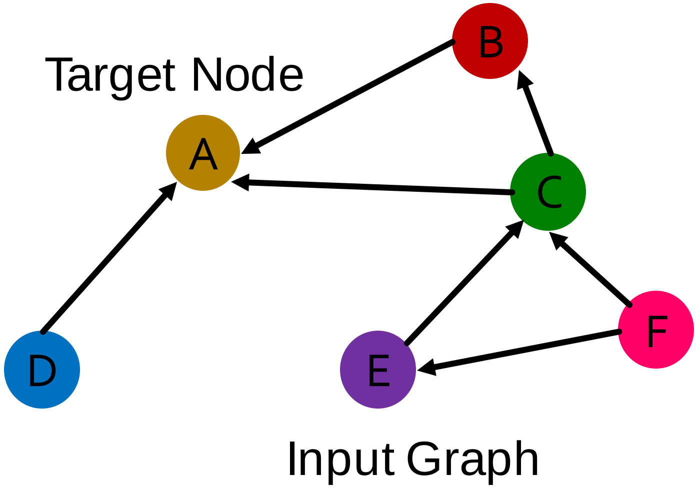
- **How to write this as Message + Aggregation?**

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



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

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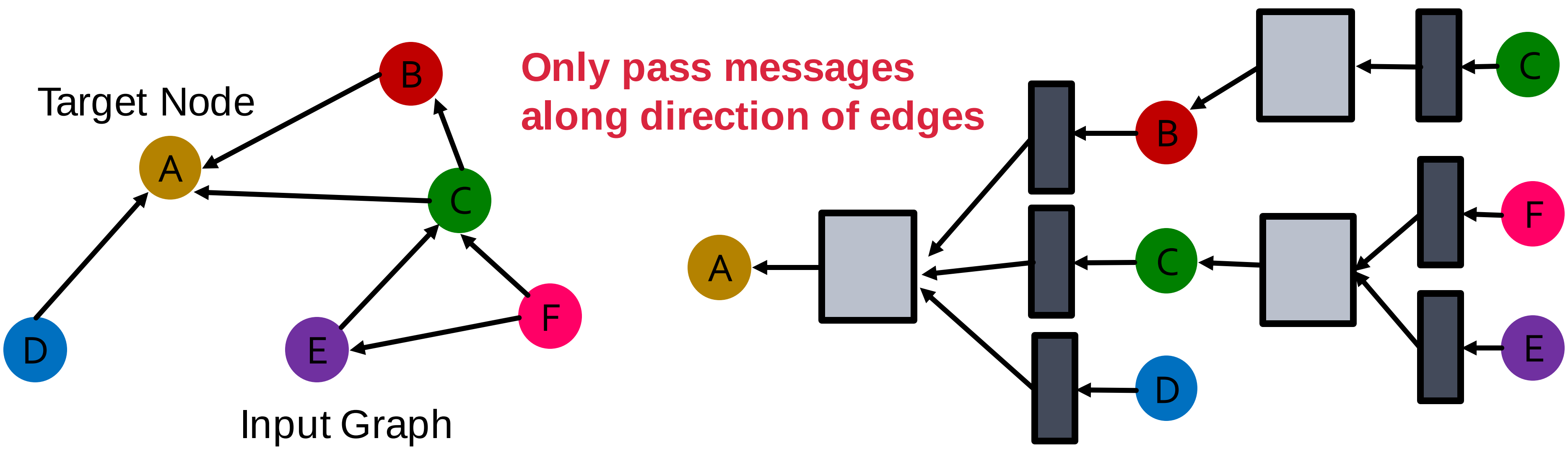
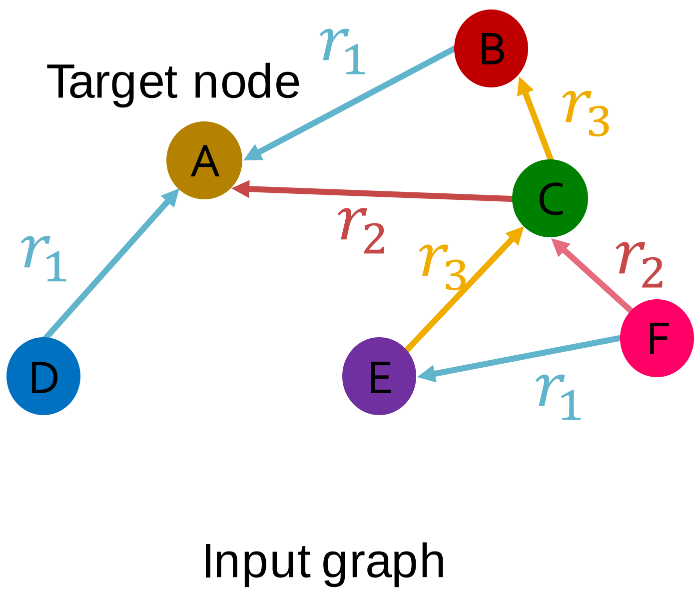


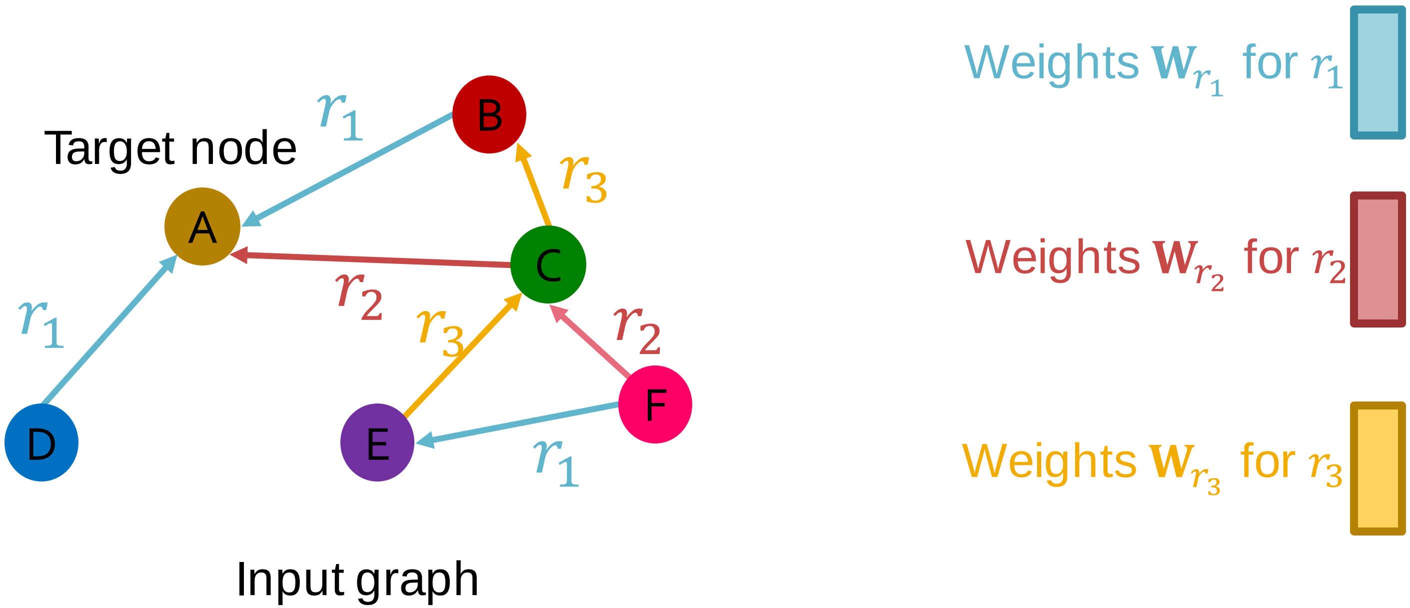
Relational GCN (1)

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



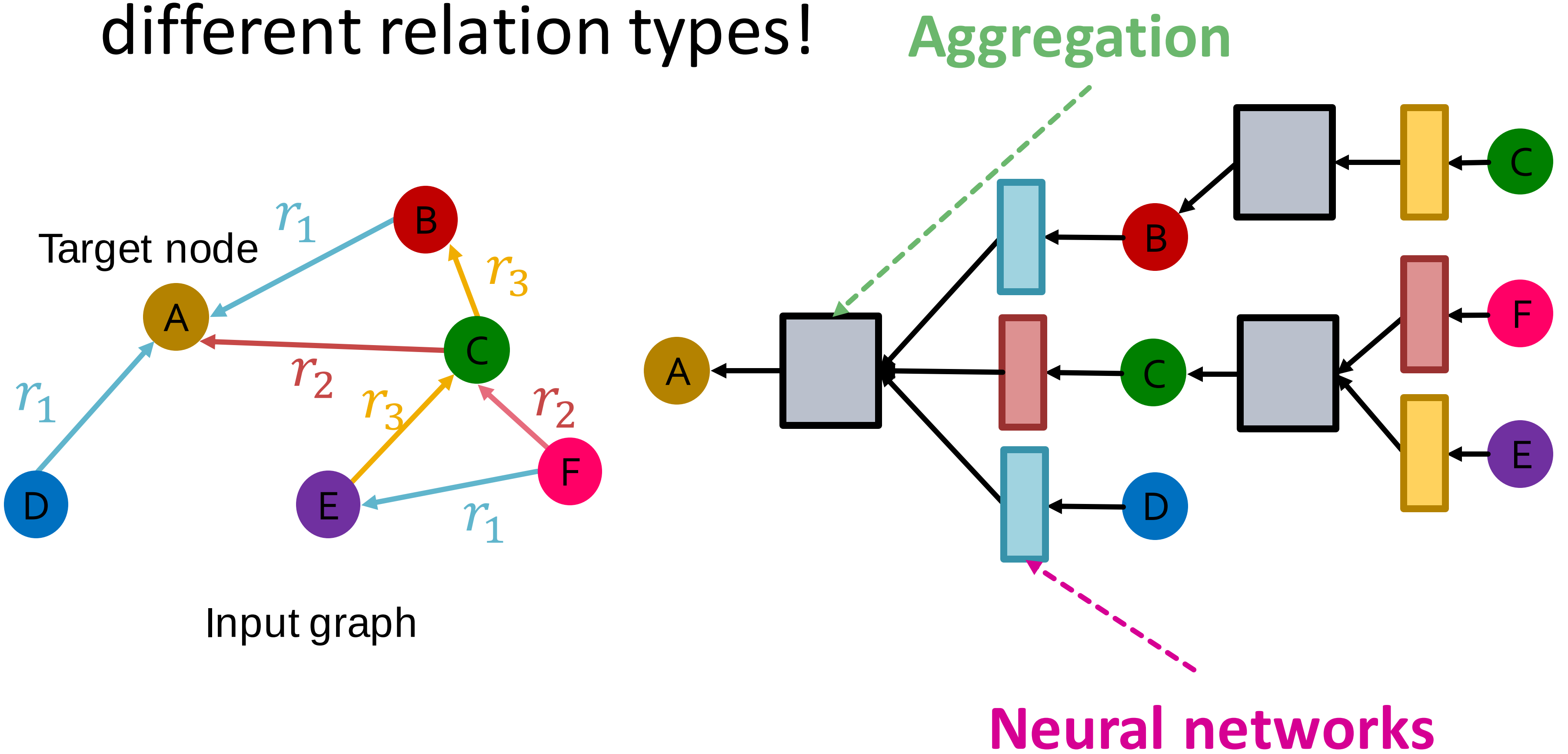
Relational GCN (2)

- **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)

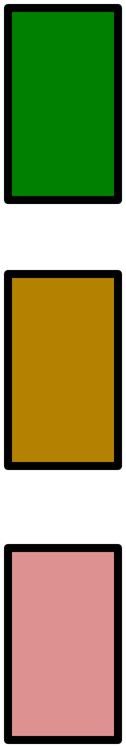
- Introduce a set of neural networks for each relation type!

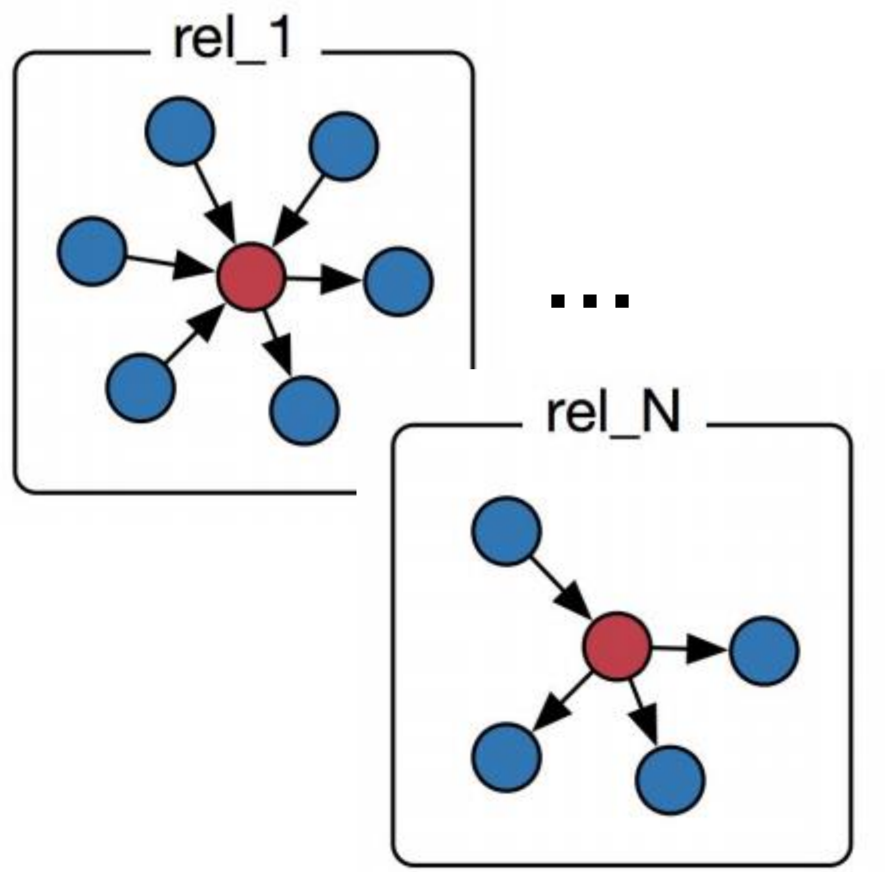
Weight for rel_1

...

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:**
  - Each neighbor of a given relation:

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

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

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

RGCN: Scalability

- Each relation has L matrices: $\mathbf{W}_r^{(1)}, \mathbf{W}_r^{(2)} \cdots \mathbf{W}_r^{(L)}$
- The size of each $\mathbf{W}_r^{(l)}$ is $d^{(l+1)} \times d^{(l)}$

$d^{(l)}$ is the hidden dimension in layer l

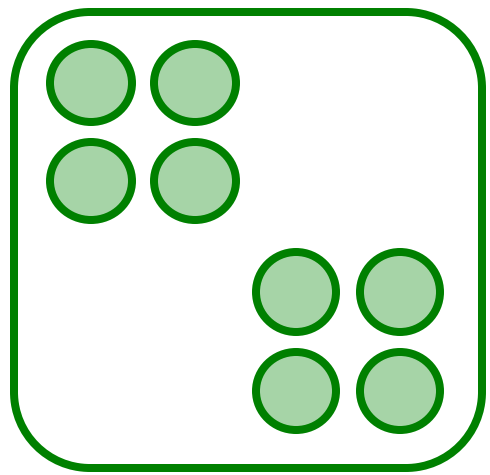
- **Rapid growth of the number of parameters w.r.t number of relations!**
  - **Overfitting becomes an issue**

- **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 $\mathbf{W}_r$

$$\mathbf{W}_r =$$



Limitation: only nearby neurons/dimensions can interact through W

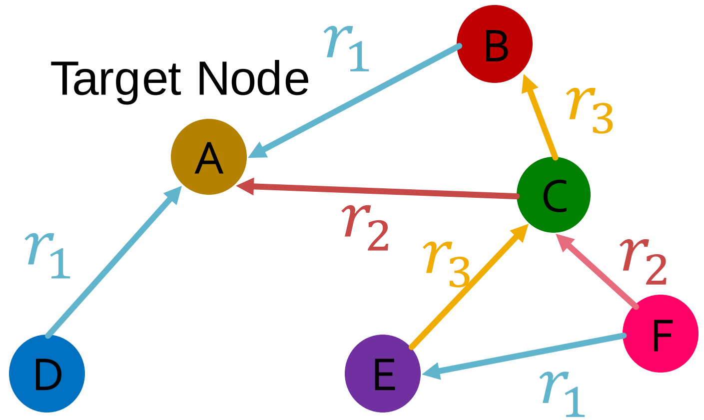
- If use B low-dimensional matrices, then # param reduces from $d^{(l+1)} \times d^{(l)}$ to $B \times \frac{d^{(l+1)}}{B} \times \frac{d^{(l)}}{B}$

(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

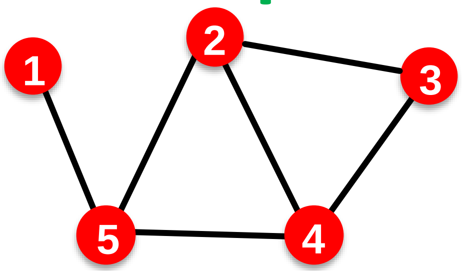
- **Goal: Predict the label of a given node**
- **RGCN** uses the representation of the final layer:
  - If we predict the class of **node A** from **k classes**
  - Take the **final layer (prediction head)**: $\mathbf{h}_A^{(L)} \in \mathbb{R}^k$, each item in $\mathbf{h}_A^{(L)}$ represents **the probability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



Input Graph

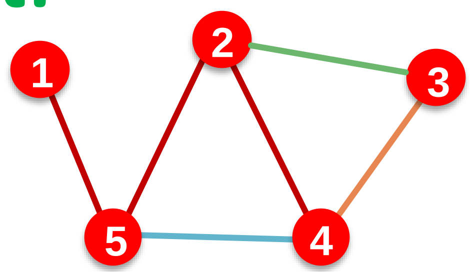
Example: Link Prediction

- **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

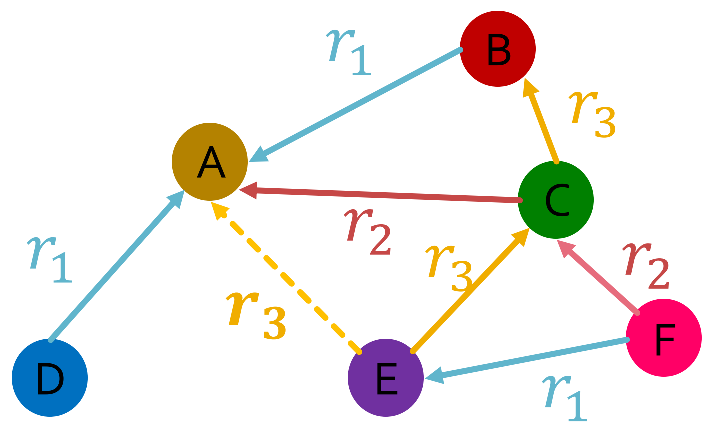
⋮

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)

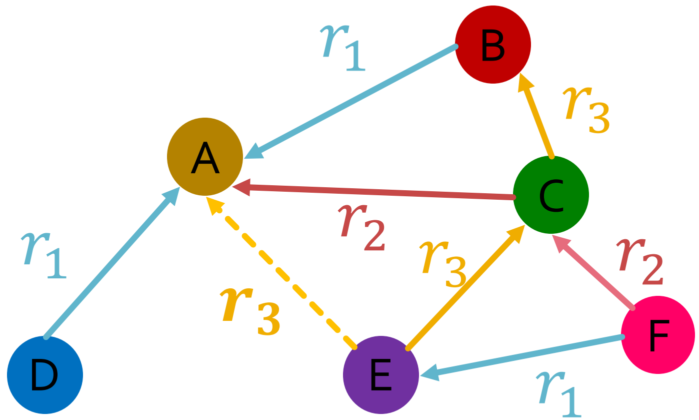
- **Assume (E, r_3, A) is training supervision edge, all the other edges are training message edges**
- **Use RGCN to score (E, r_3, A)!**
  - Take the final layer of E and A: $\mathbf{h}_E^{(L)}$ and $\mathbf{h}_A^{(L)} \in \mathbb{R}^d$
  - Relation-specific score function $f_r: \mathbb{R}^d \times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



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)**

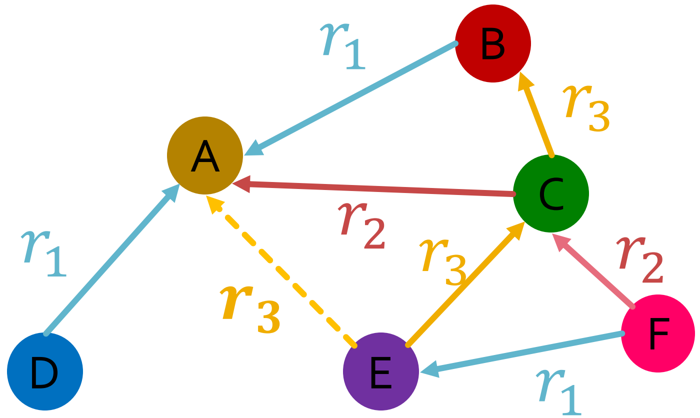
training supervision edges: (E, r_3, A)
training message edges: **all the rest existing edges (solid lines)**

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:**



Input Graph

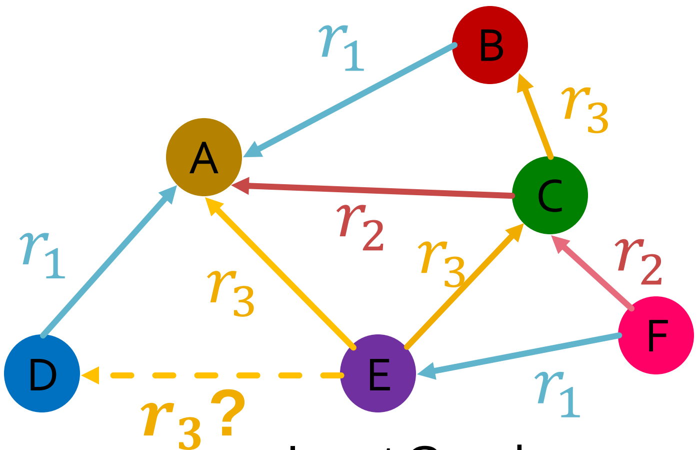
1. **Use RGCN to score the training supervision edge $(\boldsymbol{E}, \boldsymbol{r_3}, \boldsymbol{A})$**
2. **Create a negative edge by perturbing the supervision edge $(\boldsymbol{E}, \boldsymbol{r_3}, \boldsymbol{B})$**
3. **Use GNN model to score negative edge**
4. **Optimize a standard cross 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**



Input Graph

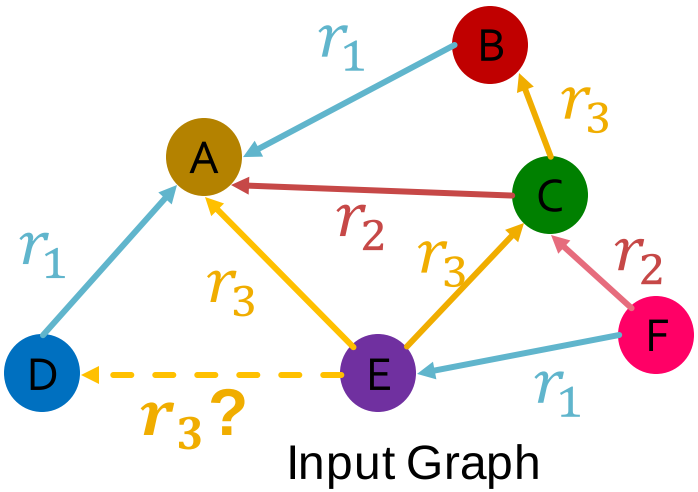
Evaluate how the model can predict the validation edges with the relation types.
Let's predict validation edge (E, r_3, D)
Intuition: the score of (E, r_3, D) should be higher than all (E, r_3, v) where (E, r_3, v) is NOT in the training message edges and training supervision edges, e.g., (E, r_3, B)

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**

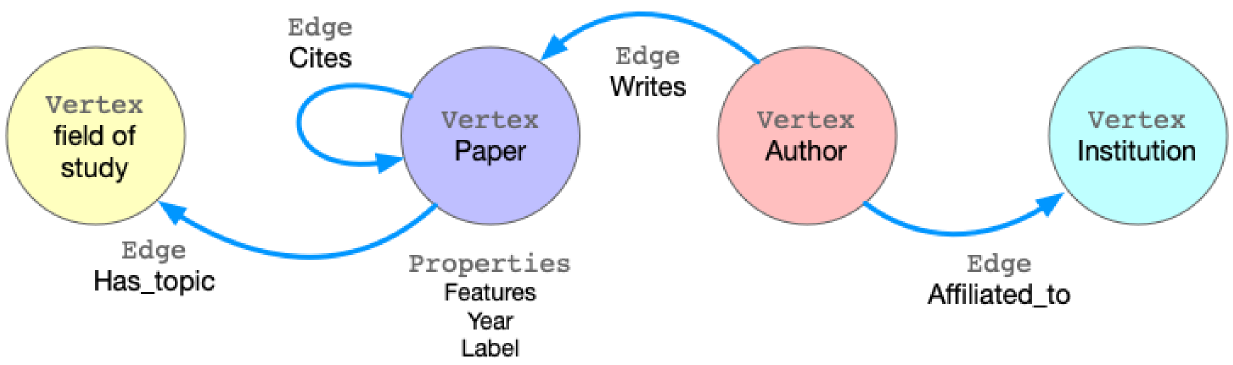


Evaluate how the model can predict the validation edges with the relation types.
Let's predict validation edge (E, r_3, D)
Intuition: the score of (E, r_3, D) should be higher than all (E, r_3, v) where (E, r_3, v) is NOT in the training message edges and training supervision edges, e.g., (E, r_3, B)

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: $1\,[RK \le k]$. Higher is better**
   2. **Reciprocal Rank: $\frac{1}{RK}$. Higher is better**

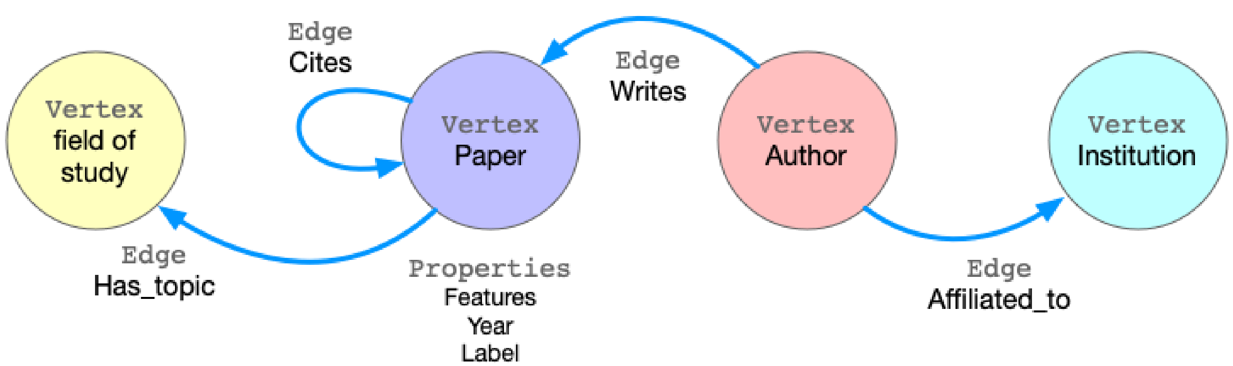
Benchmark for Heterogeneous Graphs (1)

- 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



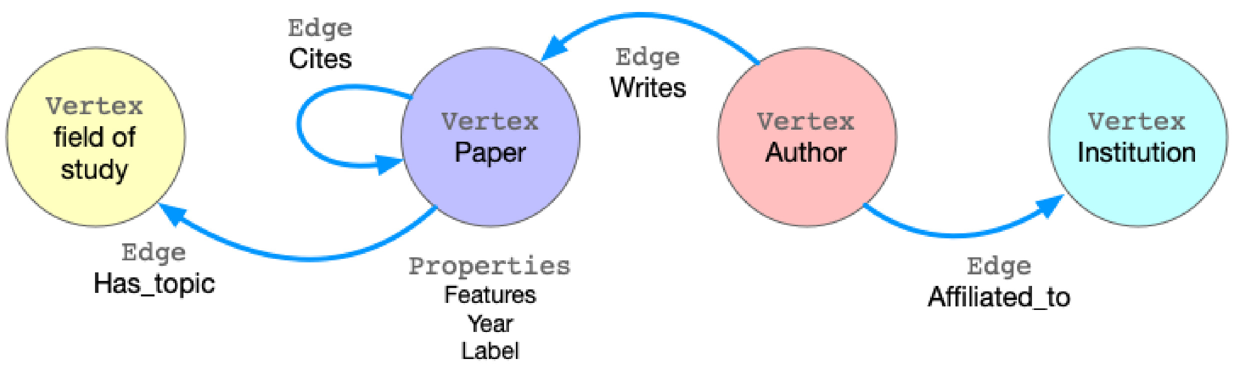
Benchmark for Heterogeneous Graphs (2)

- 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

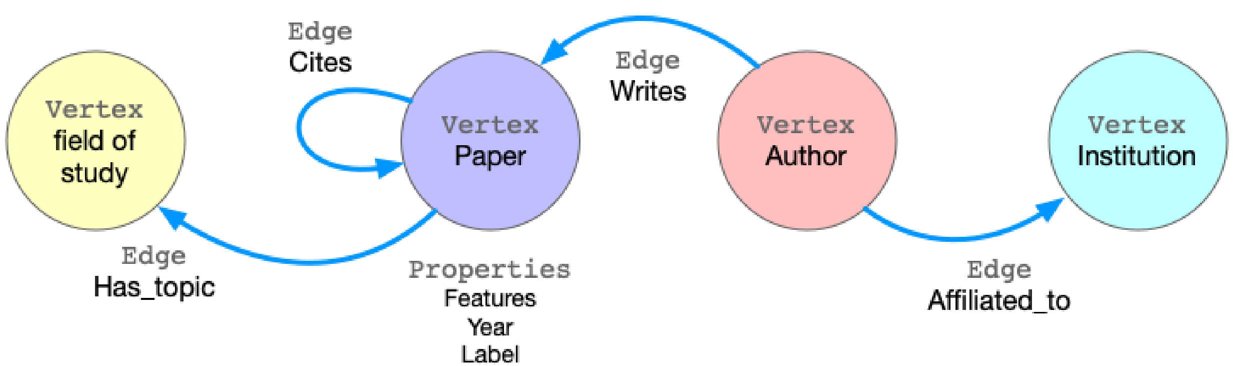


Benchmark for Heterogeneous Graphs (4)

- **Benchmark results:**

	Rank	Method	Ext. data	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
SOTA	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
R-GCN	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 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

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Recap: Graph Attention Networks

- Graph Attention Networks (GAT)

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

Attention weights

Not all node's neighbors are equally important

  - **Attention** is inspired by cognitive attention.
  - The **attention** $\boldsymbol{\alpha_{vu}}$ 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?**

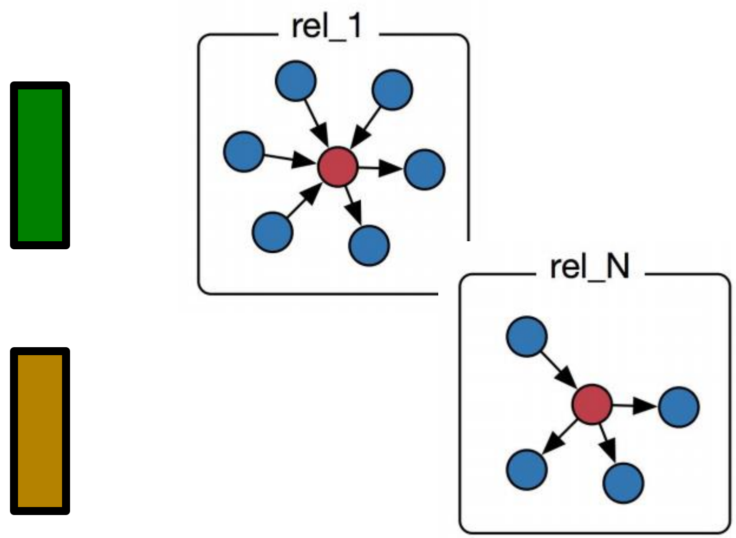
Heterogeneous Graph Transformer

- **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

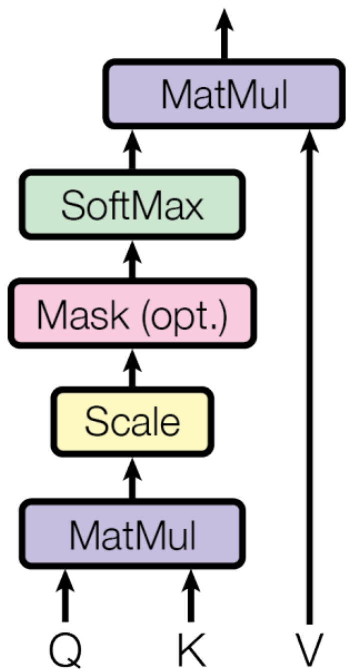


Too expensive!

Basics: Attention in Transformer

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

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



- Query: Q, Key: K, Value: V
  - Q, K, V have shape (batch_size, dim)

How do we obtain Q, K, V?

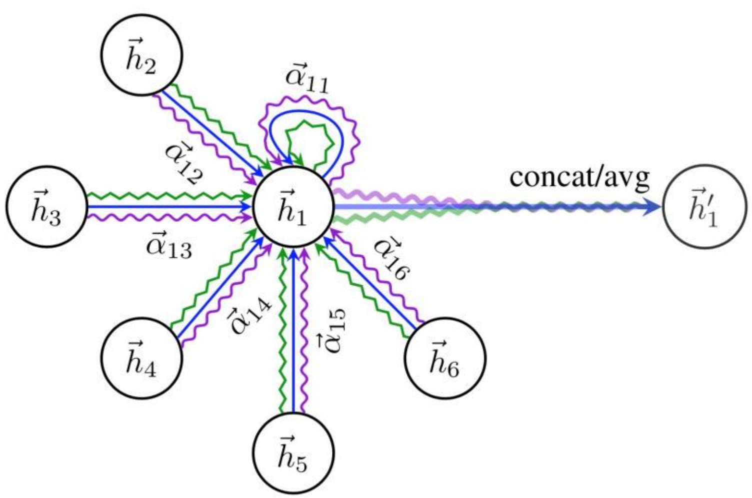
- Apply Linear layer to the input
  - $Q = Q\_Linear(X)$
  - $K = K\_Linear(X)$
  - $V = V\_Linear(X)$

Heterogeneous Mutual Attention (1)

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

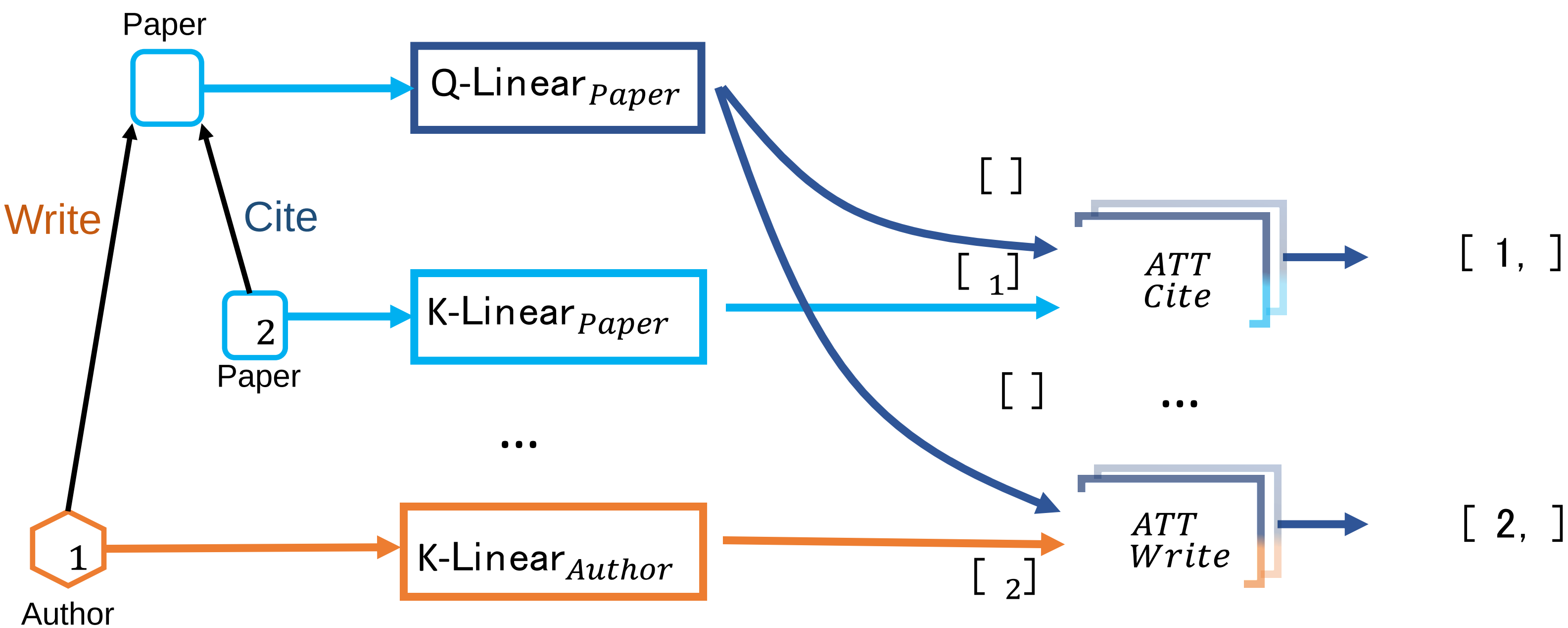
$$H^l[t] \leftarrow \text{Aggregate}_{\forall s \in N(t), \forall e \in E(s,t)} \left(\boxed{\text{Attention}(s,t)} \cdot \text{Message}(s) \right)$$

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*2*3=18 relation types -> 18 weight matrices (suppose all relation types exist)



Heterogeneous Mutual Attention (3)

- **Heterogeneous Mutual Attention:**

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

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

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

- 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**

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

We have just computed

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

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

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

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	Ziniu Hu	Paper, Code	21,173,389	Tesla K80 (12GB GPU)	Jan 26, 2021
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

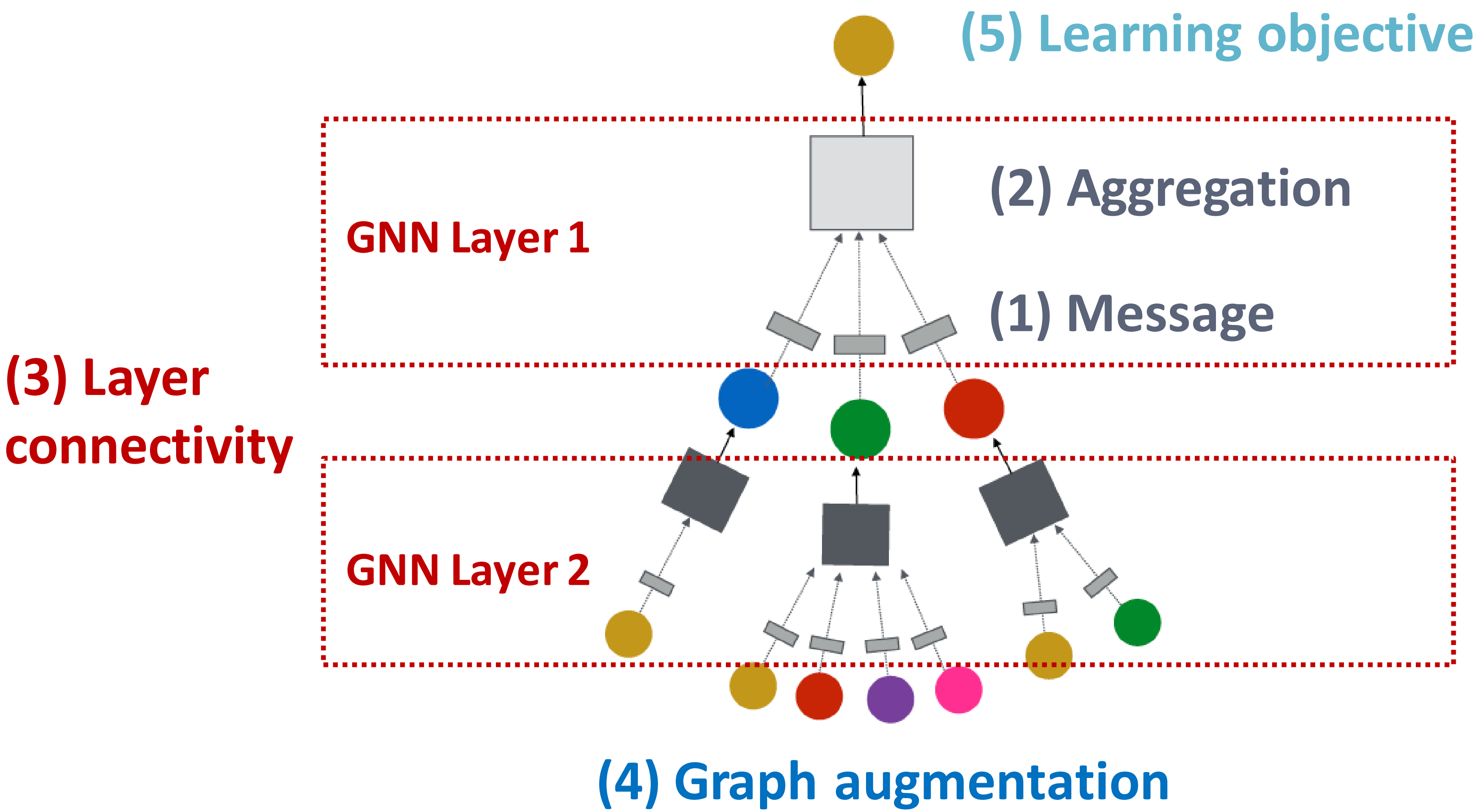
- HGT uses **much fewer parameters**, even though the attention computation is expensive, while **performs better than R-GCN**
  - Thanks to the weight decomposition over node & edge types

Stanford CS224W: Design Space of Heterogeneous GNNs

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

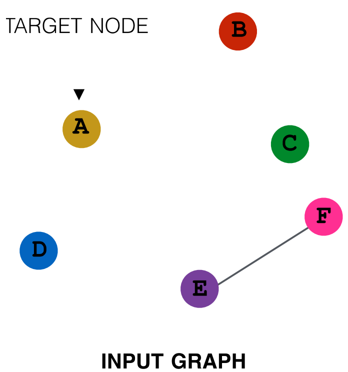
Recap: GNN Framework

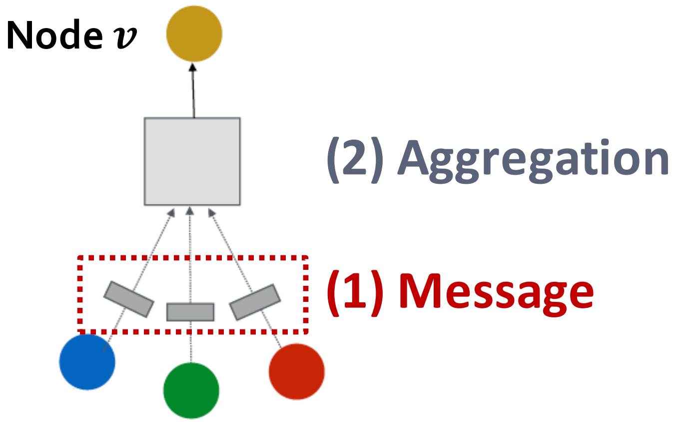
How do we extend the general GNN design space to heterogeneous graphs?



Recap: Message Computation

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

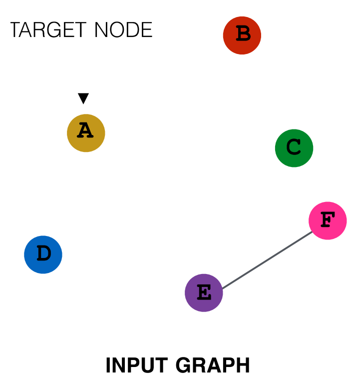
- (1) **Heterogeneous** message computation
  - **Message function:** $\mathbf{m}_u^{(l)} = \mathrm{MSG}_r^{(l)}\left(\mathbf{h}_u^{(l-1)}\right)$
    - **Observation:** A node could receive multiple types of messages. **Num of message type = Num of relation type**
    - **Idea:** Create a different message function for each relation type
      - $\mathbf{m}_u^{(l)} = \mathrm{MSG}_r^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), r = (u, e, v)$ 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 $\mathbf{m}_u^{(l)} = \mathbf{W}_r^{(l)}\mathbf{h}_u^{(l-1)}$

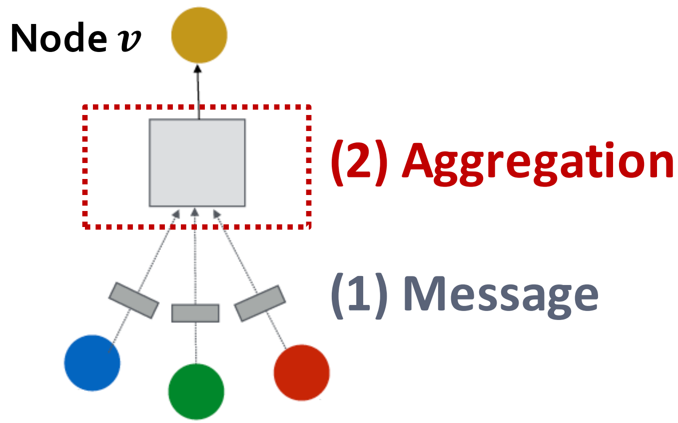
Recap: Message Aggregation

- **(2) Aggregation**
  - **Intuition:** Each node will aggregate the messages from node v's neighbors

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

  - **Example:** $\mathrm{Sum}(\cdot)$, $\mathrm{Mean}(\cdot)$ or $\mathrm{Max}(\cdot)$ aggregator
    - $\mathbf{h}_v^{(l)} = \mathrm{Sum}(\{\mathbf{m}_u^{(l)}, u \in N(v)\})$



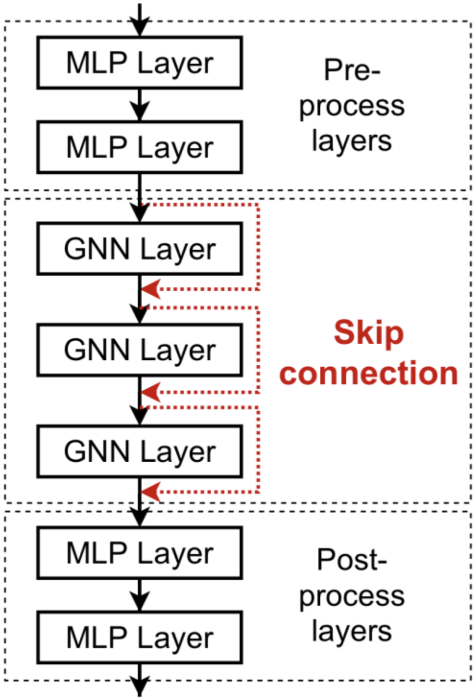


Heterogeneous Aggregation

- (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
    - $\mathbf{h}_v^{(l)} = \mathrm{AGG}_{all}^{(l)}\left(\mathrm{AGG}_r^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N_r(v)\right\}\right)\right)$
    - Given all the messages sent to a node
    - Within each message type, aggregate the messages that belongs to the edge type with $\mathrm{AGG}_r^{(l)}$
    - Aggregate across the edge types with $\mathrm{AGG}_{all}^{(l)}$
  - **Example:** $\mathbf{h}_v^{(l)} = \mathrm{Concat}\left(\mathrm{Sum}\left(\left\{\mathbf{m}_u^{(l)}, u \in N_r(v)\right\}\right)\right)$

Recap: Layer connectivity

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



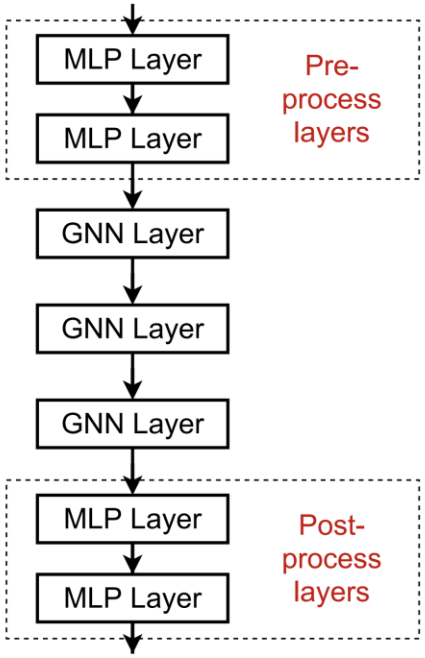
Pre-processing layers: Important when encoding node features is necessary.
E.g., when nodes represent images/text

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:

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

Edge-level prediction:

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

Graph-level prediction:

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

Heterogeneous Prediction Heads

Node-level prediction:

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

Edge-level prediction:

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

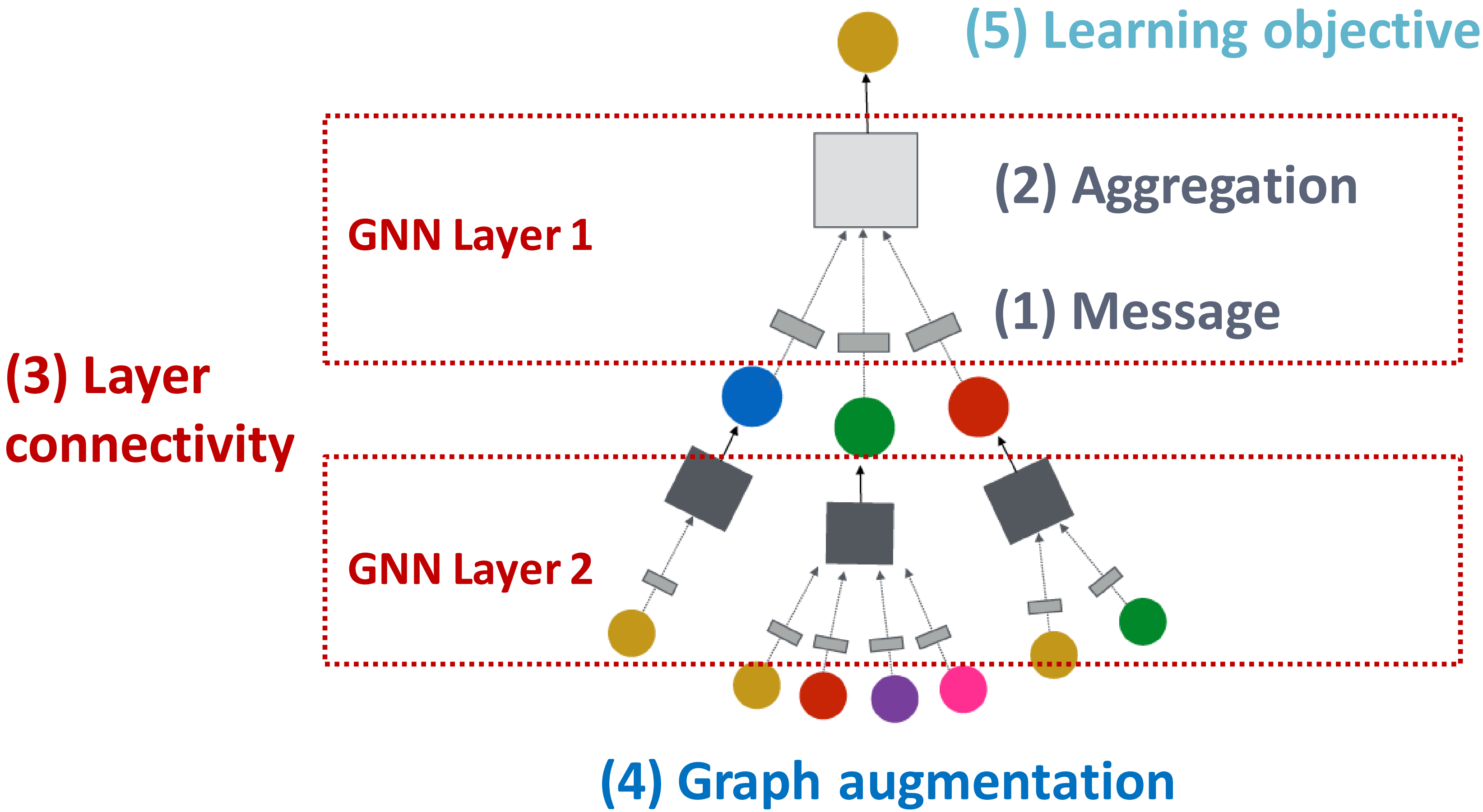
Graph-level prediction:

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

J. You, R. Ying, J. Leskovec. Design Space of Graph Neural Networks, NeurIPS 2020

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**