

Stanford CS224W: **Heterogeneous Graphs and** **Knowledge Graph Embeddings**

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



ANNOUNCEMENTS

- **Colab 2 due today**
 - When you submit, you should get 0/0 on your assignment – this is because our test cases are hidden and will be graded after the assignment deadline
 - However, we have a simple autograder to make sure you are zipping files correctly: you should *not* see any errors (e.g., ModuleNotFoundError)
 - See details in Ed announcement ("Colab 2 out")
- **HW1 grades released after class**

CS224W: Machine Learning with Graphs

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ANNOUNCEMENTS

- **NEW: Group OH for HW2 (due Thursday 10/28)**
 - In response to student feedback, we will hold some group OH
 - **(1) Alex's OH: Tuesday 10/26 3:30-5:30pm**
 - **(2) Giray's OH: Wednesday 10/27 4-6pm**
 - ~40 minutes per question, everyone in the Zoom room together, Alex and Giray will walk through the problem and take questions – will be recorded
 - Other OHs will remain 1:1 so that students with specific questions can still get help / share screen

CS224W: Machine Learning with Graphs

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Today: Heterogeneous Graphs

- **Goal:**
 - So far we only handle graphs with one edge type.
 - How to handle (directed) graphs with multiple edge types (a.k.a heterogeneous graphs)?
- **Heterogeneous Graphs**
 - Relational GCNs
 - Knowledge Graphs
 - Embeddings for KG Completion

Stanford CS224W: Heterogeneous Graphs and Relational GCN (RGCN)

CS224W: Machine Learning with Graphs

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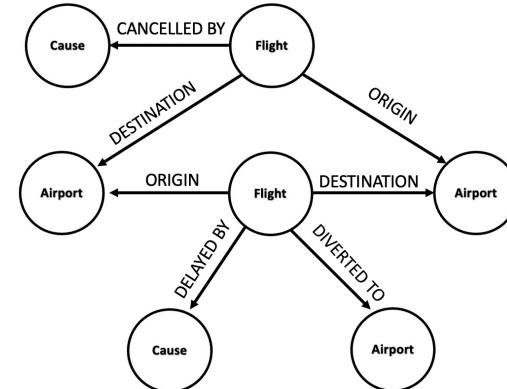
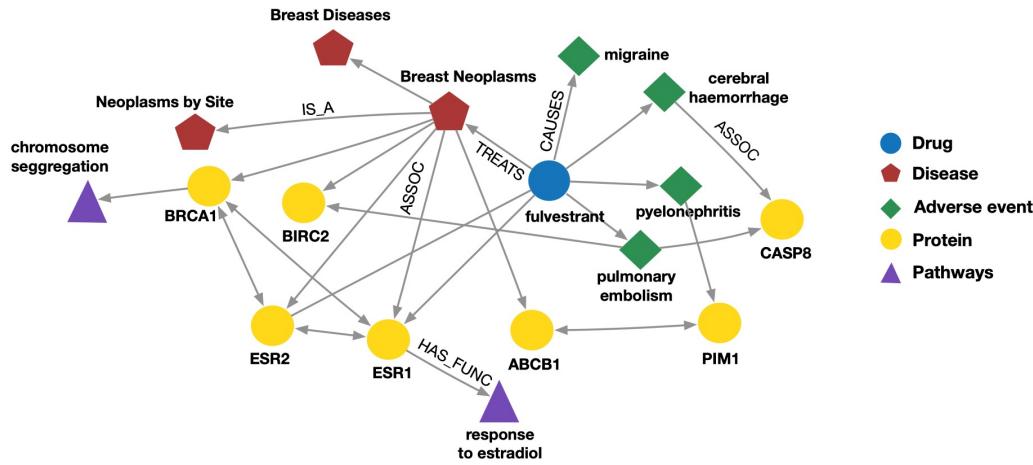
Heterogeneous Graphs

- A heterogeneous graph is defined as

$$G = (V, E, R, T)$$

- Nodes with node types $v_i \in V$
- Edges with relation types $(v_i, r, v_j) \in E$
- Node type $T(v_i)$
- Relation type $r \in R$

Many Graphs are Heterogeneous Graphs (1)



Biomedical Knowledge Graphs

Example node: Migraine

Example edge: (fulvestrant, Treats, Breast Neoplasms)

Example node type: Protein

Example edge type (relation): Causes

Event Graphs

Example node: SFO

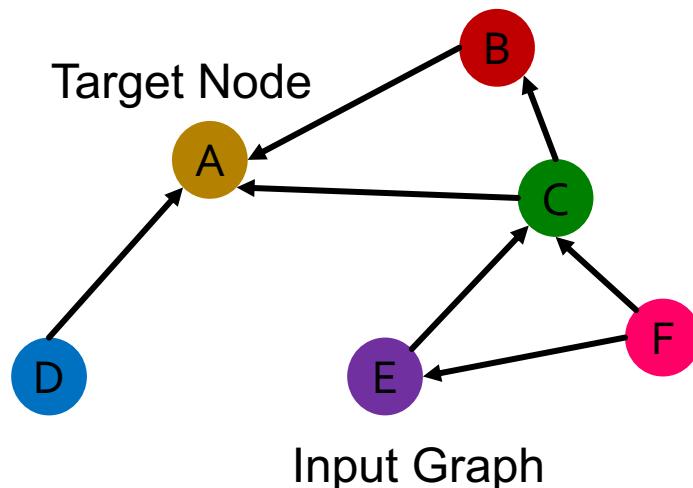
Example edge: (UA689, Origin, LAX)

Example node type: Flight

Example edge type (relation): Destination

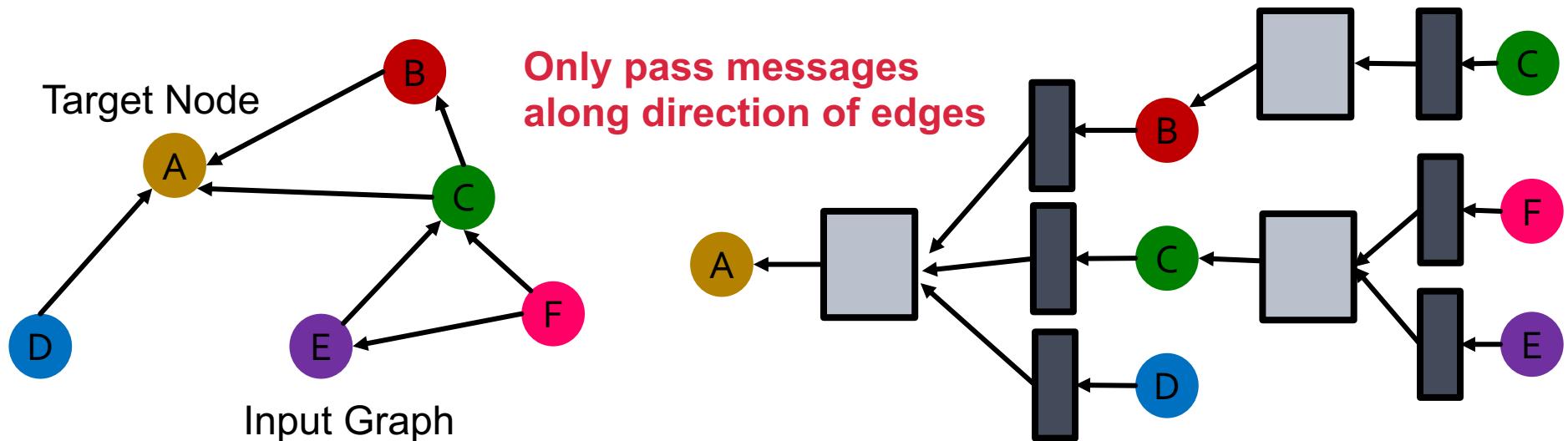
Relational GCN

- 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?



Recap: A Single GNN Layer

- A single GNN layer:

- (1) **Message**: each node computes a message

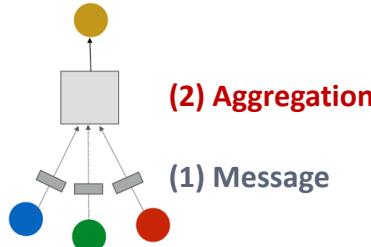
$$\mathbf{m}_u^{(l)} = \text{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$$

- (2) **Aggregation**: aggregate messages from neighbors

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

- **Nonlinearity (activation)**: Adds expressiveness

- Often written as $\sigma(\cdot)$: ReLU(\cdot), Sigmoid(\cdot) , ...
 - Can be added to **message or aggregation**



Recap: Classical GNN Layers: GCN (1)

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

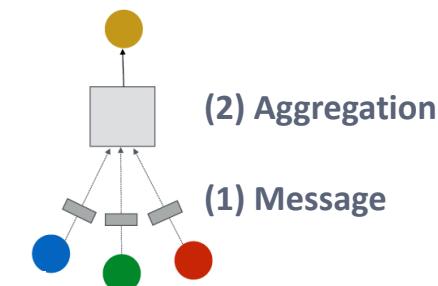
$$\mathbf{h}_v^{(l)} = \sigma \left(\mathbf{W}^{(l)} \sum_{u \in N(v)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|} \right)$$

- How to write this as Message + Aggregation?

Message

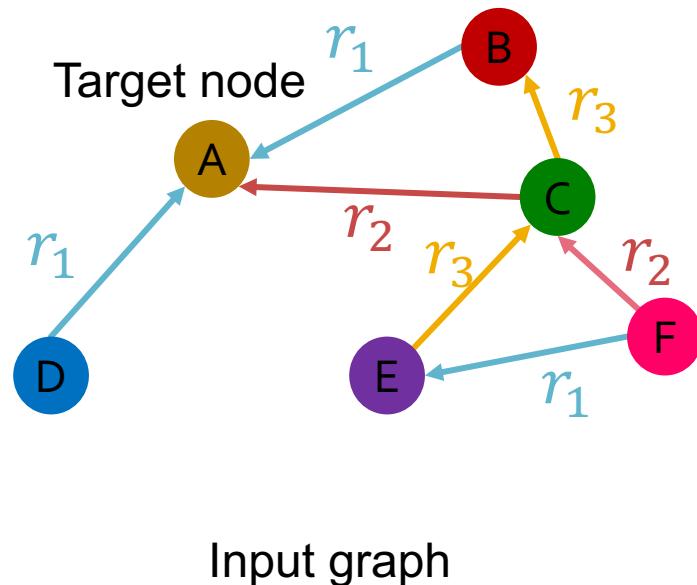
$$\mathbf{h}_v^{(l)} = \sigma \left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|} \right)$$

Aggregation



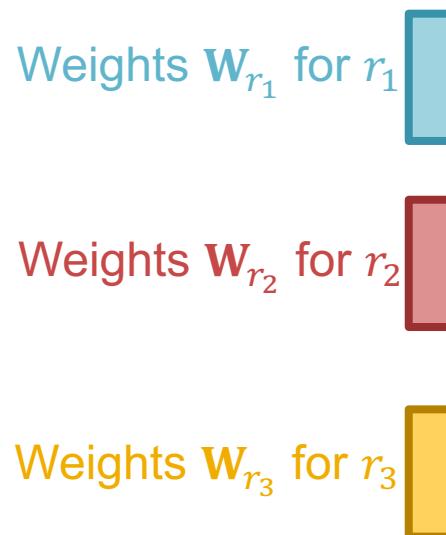
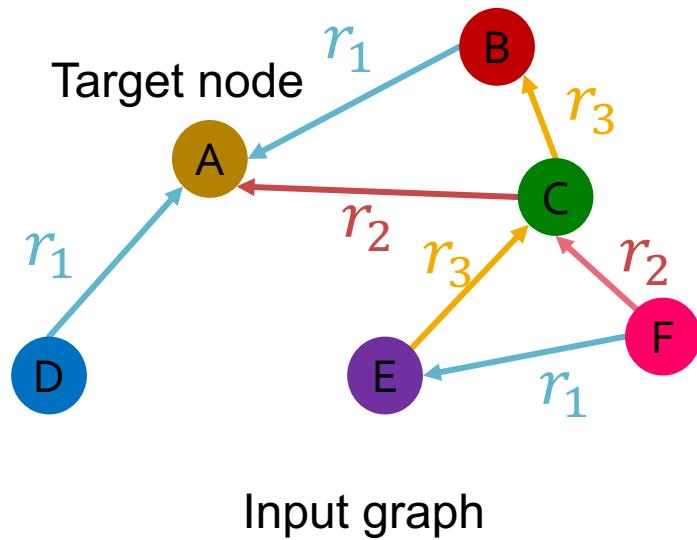
Relational GCN (1)

- What if the graph has multiple relation types?



Relational GCN (2)

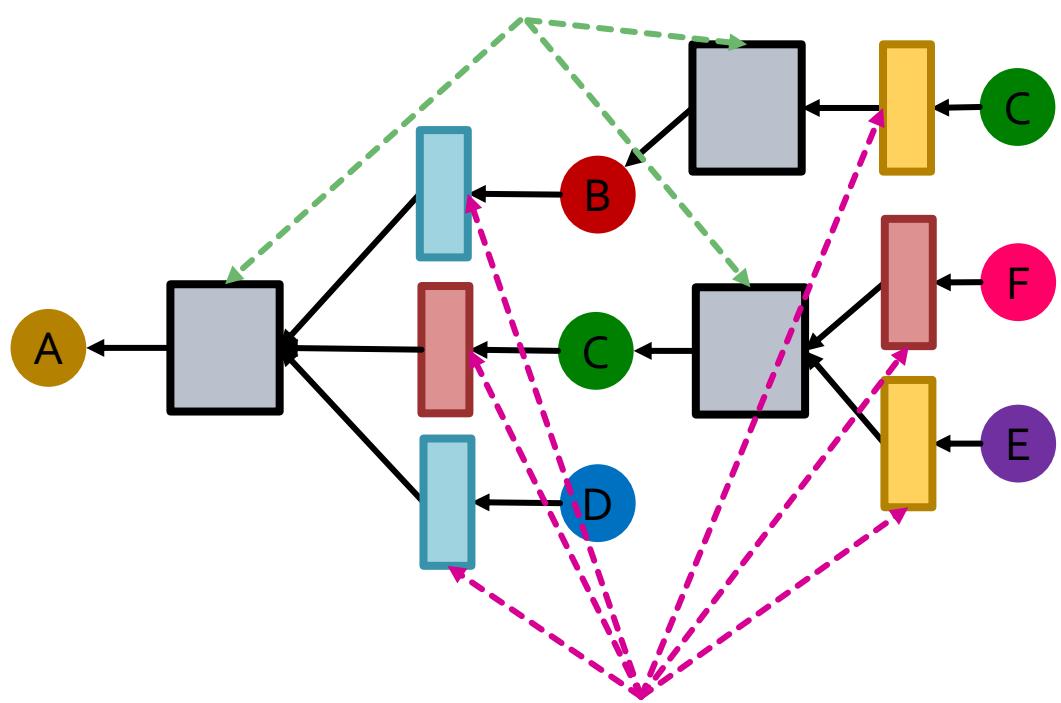
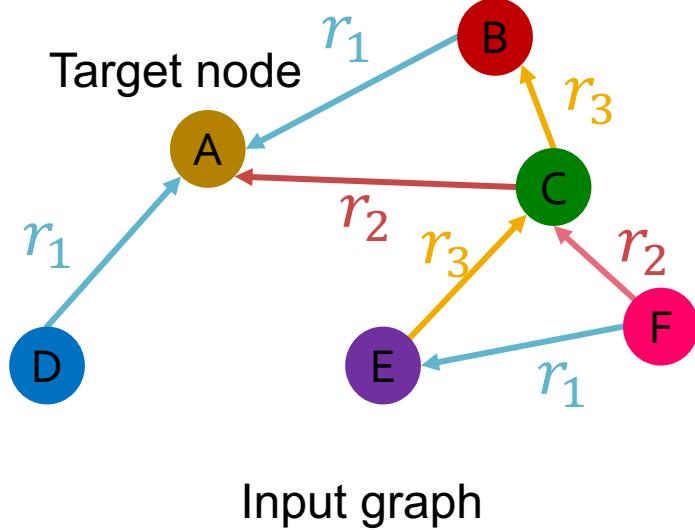
- What if the graph has **multiple relation types**?
- Use different neural network weights for different relation types.



Relational GCN (3)

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

Aggregation



Neural networks

Relational GCN: Definition

- Relational GCN (RGCN):

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

- How to write this as Message + Aggregation?

- Message:

- Each neighbor of a given relation:

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

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

- 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

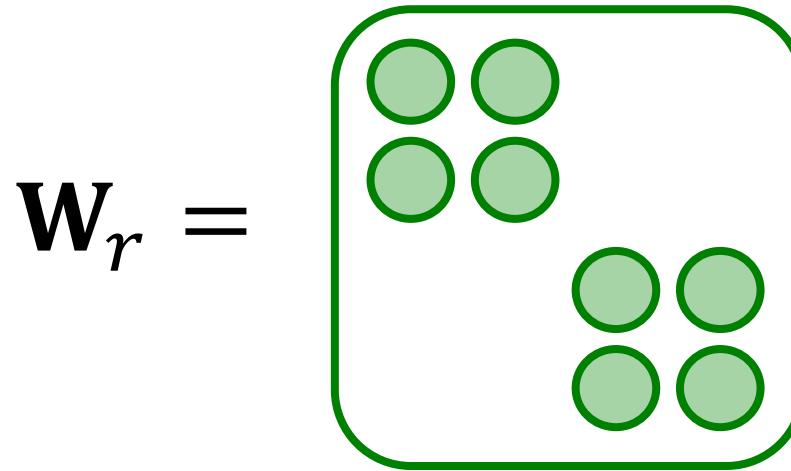
$$\mathbf{h}_v^{(l+1)} = \sigma \left(\text{Sum} \left(\left\{ \mathbf{m}_{u,\mathbf{r}}^{(l)}, u \in N(v) \right\} \cup \left\{ \mathbf{m}_v^{(l)} \right\} \right) \right)$$

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 # parameters growth w.r.t # 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 \mathbf{W}

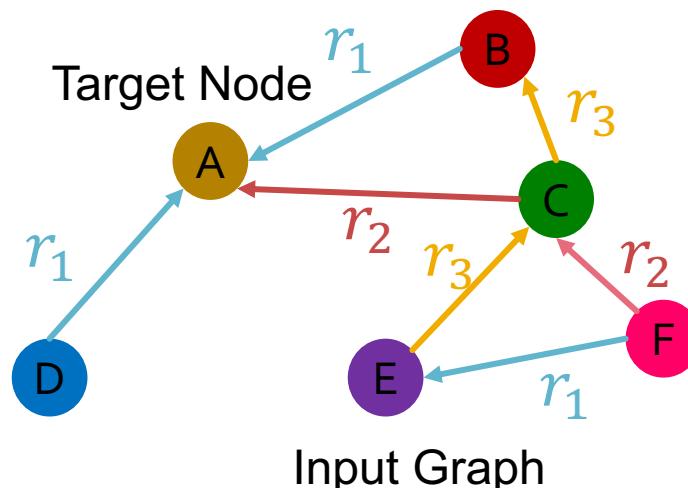
- If use B low-dimensional matrices, then # param reduces from $d^{(l+1)} \times d^{(l)}$ to $B \times \frac{d^{(l+1)}}{B} \times \frac{d^{(l)}}{B}$.

(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.

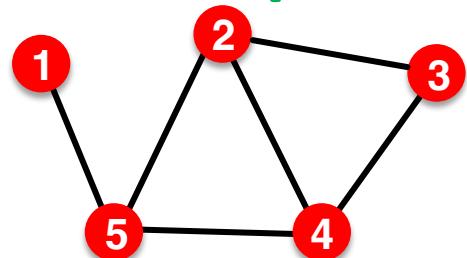
Example: Entity/Node Classification

- **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**.

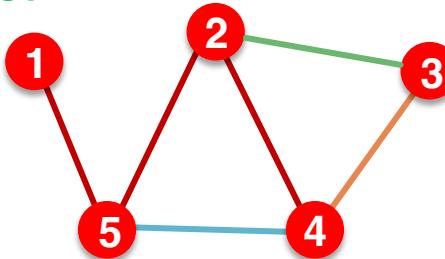


Example: Link Prediction

Link prediction split:



Split



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

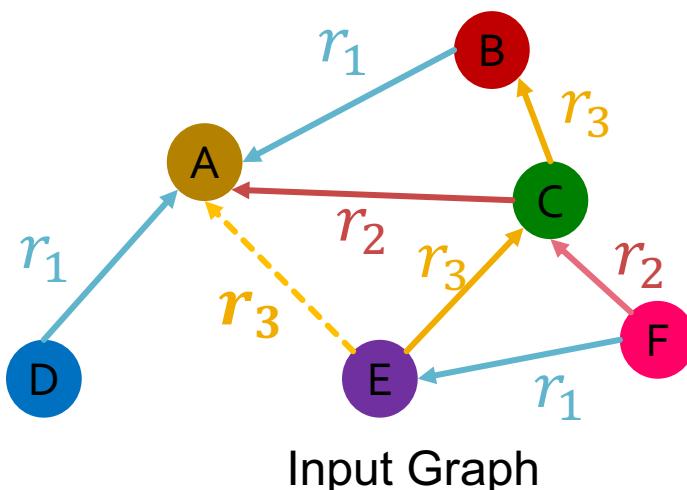
Validation edges for r_n

Test edges for r_n

Training message edges
Training supervision edges
Validation edges
Test edges

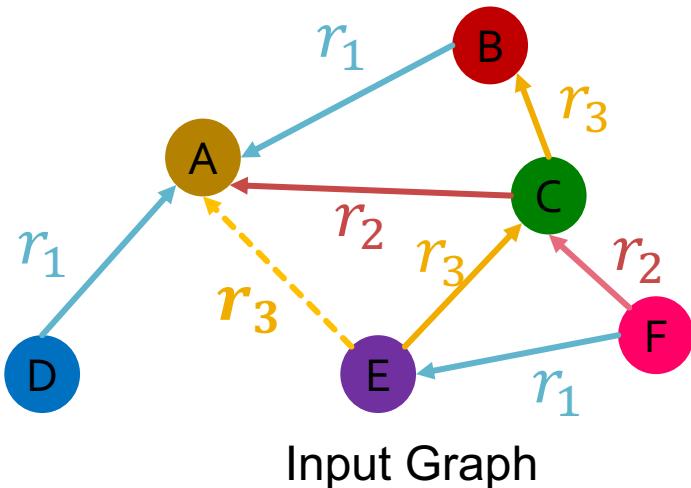
RGCN for Link Prediction (1)

- 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 $f_{r_i}: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$
 - 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)

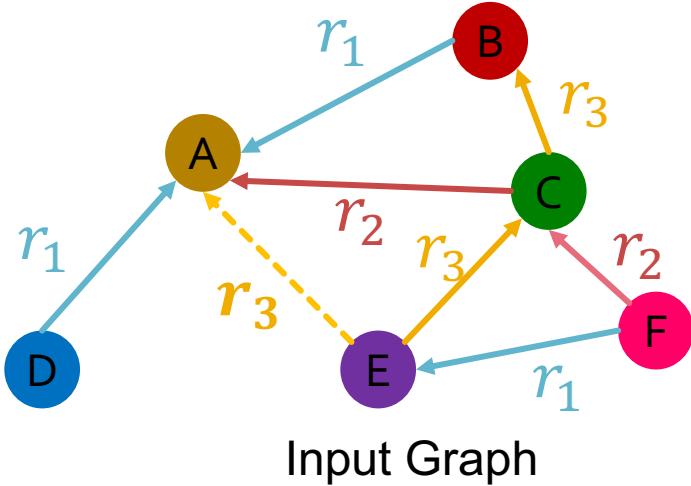
training supervision edges: (E, r_3, A)
training message edges: all the rest
existing edges (solid lines)

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**

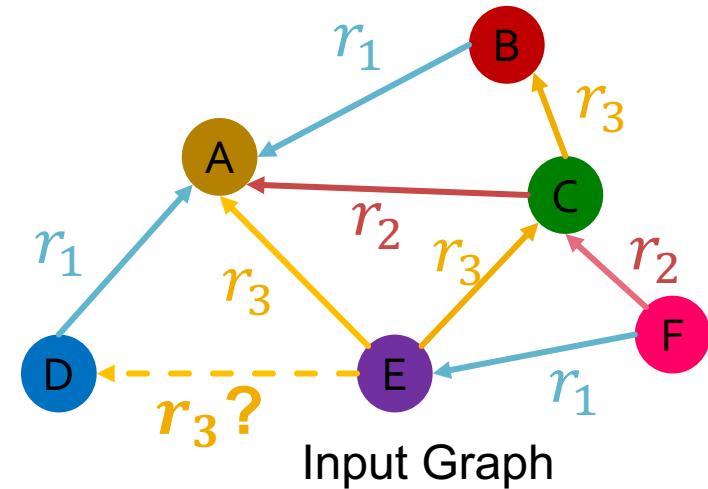
$$\ell = -\log \sigma(f_{r_3}(h_E, h_A)) - \log(1 - \sigma(f_{r_3}(h_E, h_B)))$$

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

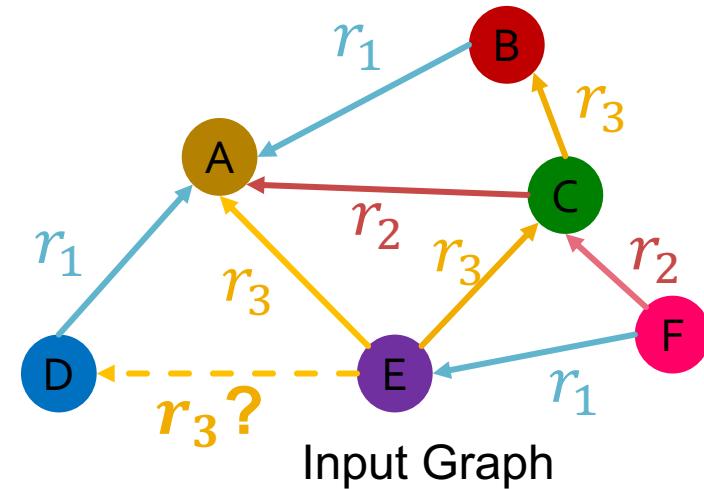
edges: all existing edges (solid lines)

(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

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.)

Stanford CS224W: Knowledge Graphs: KG Completion with Embeddings

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

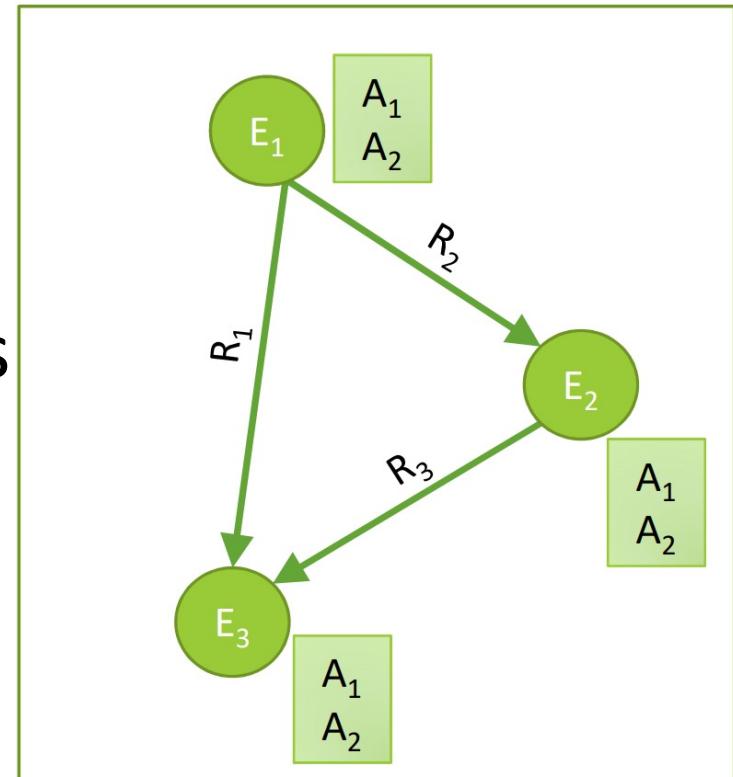
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Knowledge Graphs (KG)

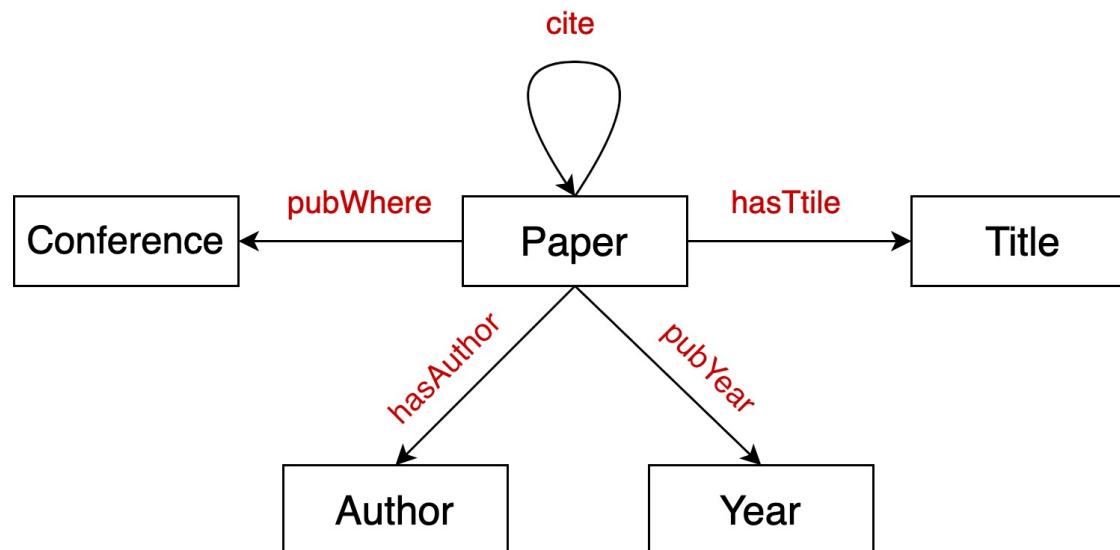
Knowledge in graph form:

- Capture entities, types, and relationships
- Nodes are **entities**
- Nodes are labeled with their **types**
- Edges between two nodes capture **relationships** between entities
- **KG is an example of a heterogeneous graph**



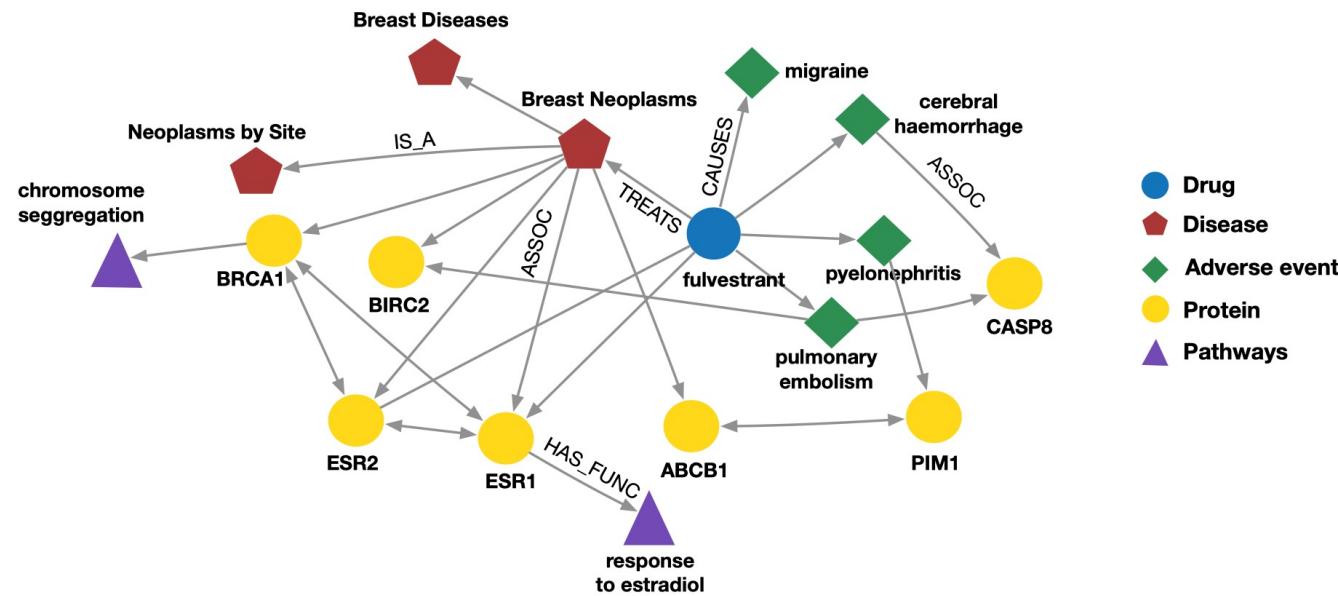
Example: Bibliographic Networks

- **Node types:** paper, title, author, conference, year
- **Relation types:** pubWhere, pubYear, hasTitle, hasAuthor, cite



Example: Bio Knowledge Graphs

- **Node types:** drug, disease, adverse event, protein, pathways
- **Relation types:** has_func, causes, assoc, treats, is_a



Knowledge Graphs in Practice

Examples of knowledge graphs

- Google Knowledge Graph
- Amazon Product Graph
- Facebook Graph API
- IBM Watson
- Microsoft Satori
- Project Hanover/Literome
- LinkedIn Knowledge Graph
- Yandex Object Answer

Applications of Knowledge Graphs

■ Serving information

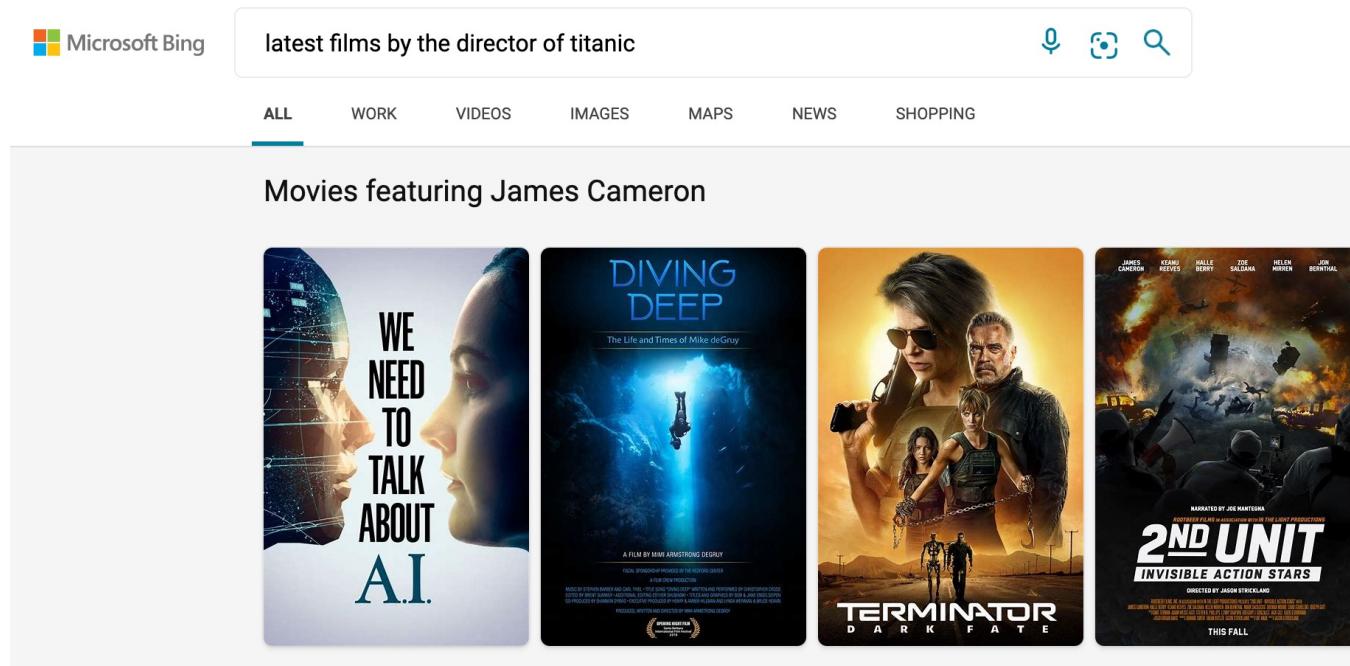


Image credit: Bing

Applications of Knowledge Graphs

■ Question answering and conversation agents

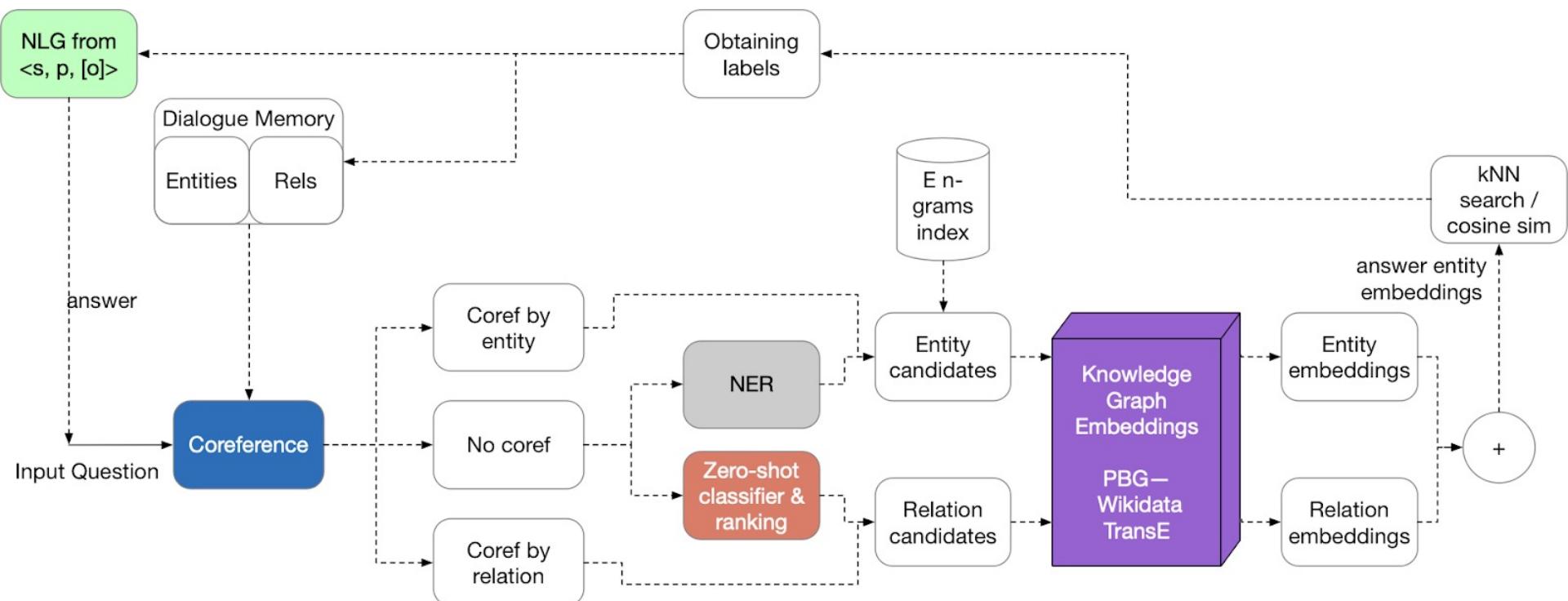


Image credit: [Medium](#)

Knowledge Graph Datasets

- **Publicly available KGs:**
 - FreeBase, Wikidata, Dbpedia, YAGO, NELL, etc.
- **Common characteristics:**
 - **Massive**: millions of nodes and edges
 - **Incomplete**: many true edges are missing

Given a massive KG,
enumerating all the
possible facts is
intractable!



Can we predict plausible
BUT missing links?

Example: Freebase



■ Freebase

- ~80 million **entities**
- ~38K **relation types**
- ~3 billion **facts/triples**

93.8% of persons from Freebase have no place of birth and 78.5% have no nationality!

■ Datasets: FB15k/FB15k-237

- A **complete** subset of Freebase, used by researchers to learn KG models

Dataset	Entities	Relations	Total Edges
FB15k	14,951	1,345	592,213
FB15k-237	14,505	237	310,079

[1] Paulheim, Heiko. "Knowledge graph refinement: A survey of approaches and evaluation methods." *Semantic web* 8.3 (2017): 489-508.

[2] Min, Bonan, et al. "Distant supervision for relation extraction with an incomplete knowledge base." *Proceedings of the 2013 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*. 2013.

Stanford CS224W: Knowledge Graph Completion: TransE, TransR, DistMul, ComplEx

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>

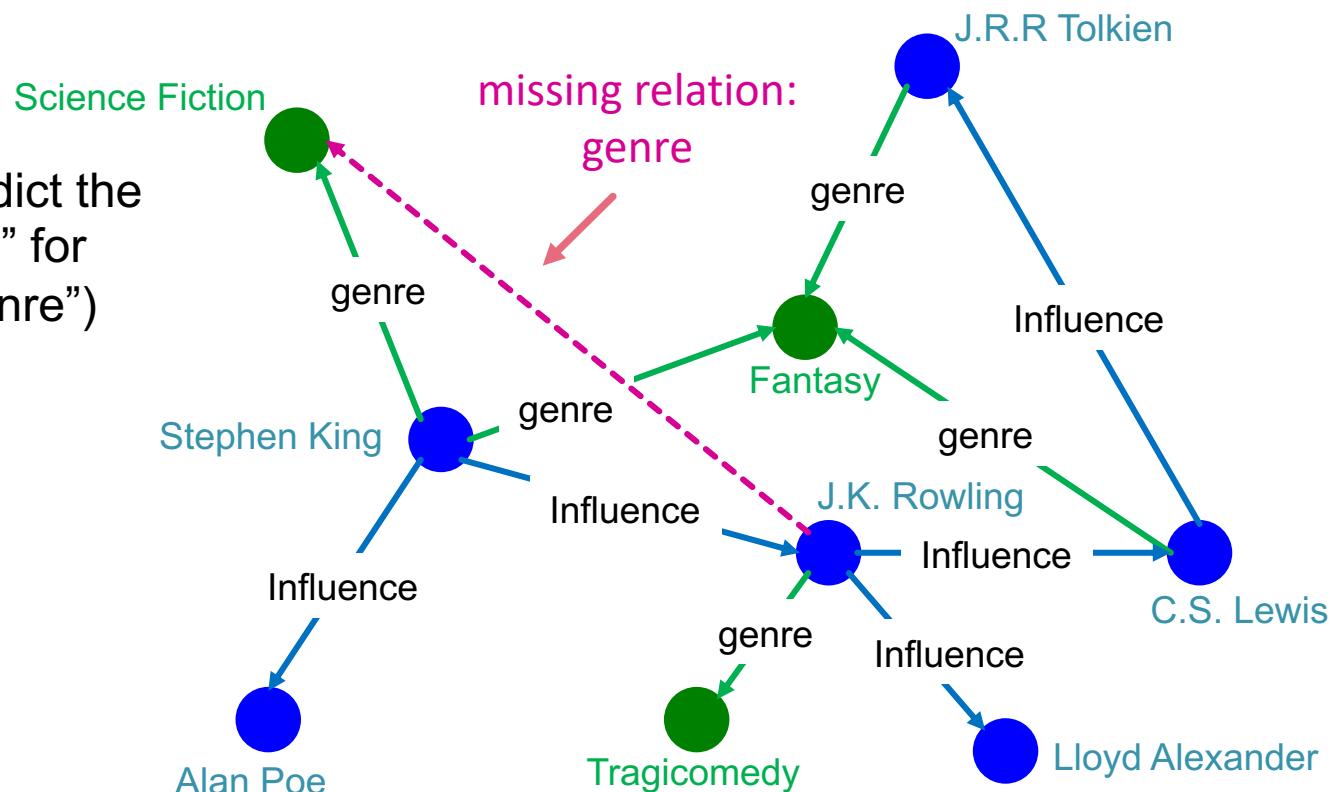


KG Completion Task

Given an enormous KG, can we complete the KG?

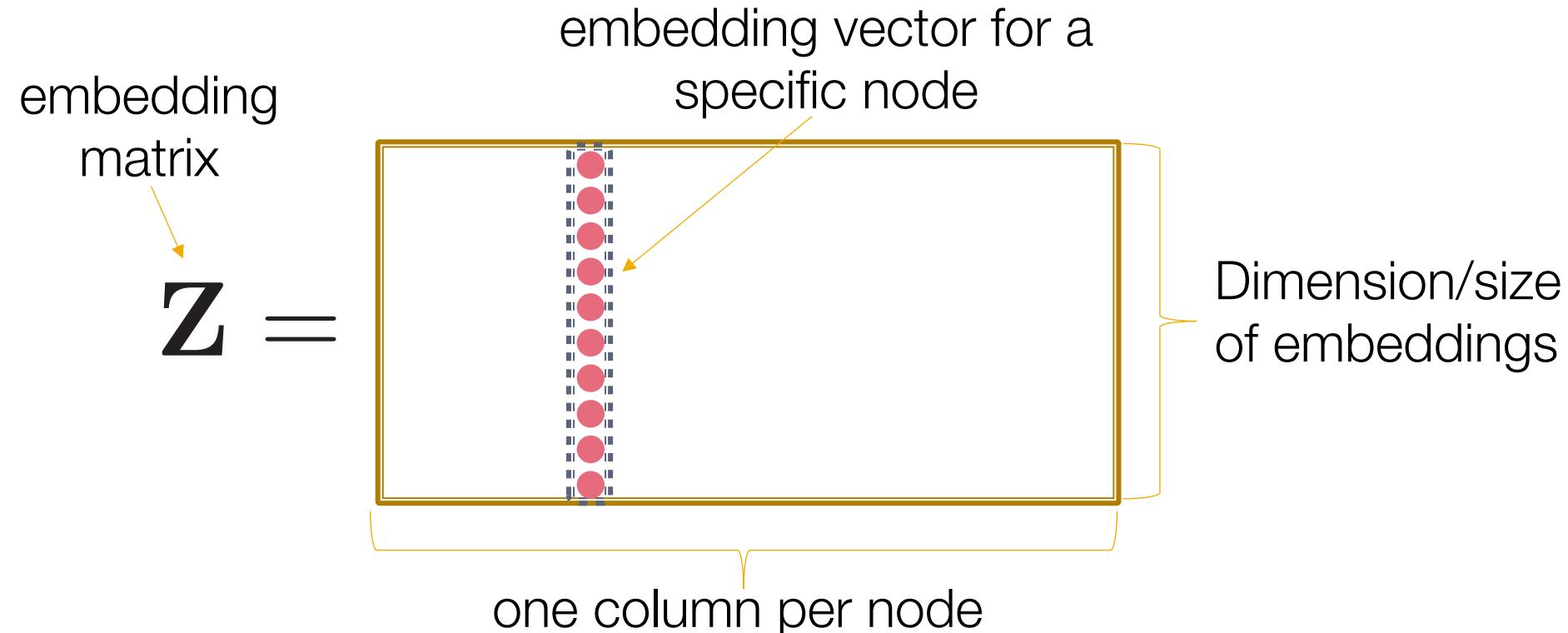
- For a given (**head**, **relation**), we predict missing **tails**.
 - (Note this is slightly different from link prediction task)

Example task: predict the tail “**Science Fiction**” for (“**J.K. Rowling**”, “genre”)



Recap: “Shallow” Encoding

- Simplest encoding approach: **encoder is just an embedding-lookup**



KG Representation

- Edges in KG are represented as **triples** (h, r, t)
 - head (h) has **relation** (r) with tail (t)
- **Key Idea:**
 - Model entities and relations in the embedding/vector space \mathbb{R}^d .
 - Associate entities and relations with **shallow embeddings**
 - **Note we do not learn a GNN here!**
 - Given a true triple (h, r, t) , the goal is that the **embedding of (h, r) should be close** to the **embedding of t** .
 - How to embed (h, r) ?
 - How to define closeness?

TransE

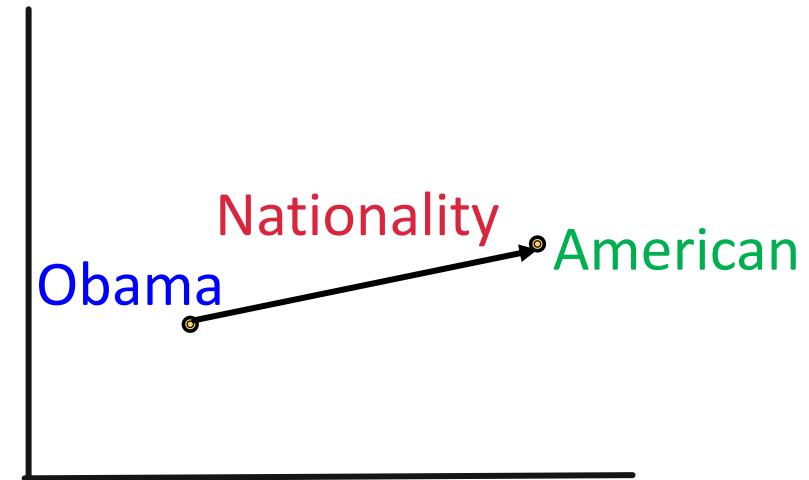
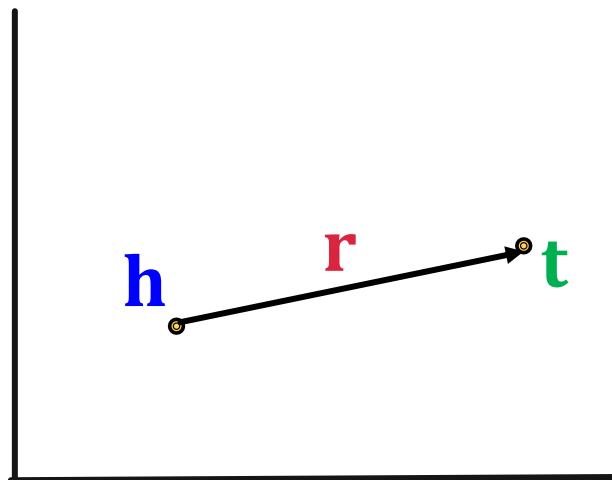
- **Translation Intuition:**

For a triple (h, r, t) , $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^d$,

embedding vectors will appear in boldface

$\mathbf{h} + \mathbf{r} \approx \mathbf{t}$ if the given fact is true
 else $\mathbf{h} + \mathbf{r} \neq \mathbf{t}$

Scoring function: $f_r(h, t) = -||\mathbf{h} + \mathbf{r} - \mathbf{t}||$



TransE Learning Algorithm

Algorithm 1 Learning TransE

input Training set $S = \{(h, \ell, t)\}$, entities and rel. sets E and L , margin γ , embeddings dim. k .

```
1: initialize  $\ell \leftarrow \text{uniform}(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$  for each  $\ell \in L$ 
2:  $\ell \leftarrow \ell / \|\ell\|$  for each  $\ell \in L$ 
3:  $e \leftarrow \text{uniform}(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$  for each entity  $e \in E$ 
4: loop
5:    $e \leftarrow e / \|e\|$  for each entity  $e \in E$ 
6:    $S_{batch} \leftarrow \text{sample}(S, b)$  // sample a minibatch of size  $b$ 
7:    $T_{batch} \leftarrow \emptyset$  // initialize the set of pairs of triplets
8:   for  $(h, \ell, t) \in S_{batch}$  do
9:      $(h', \ell, t') \leftarrow \text{sample}(S'_{(h, \ell, t)})$  // sample a corrupted triplet
10:     $T_{batch} \leftarrow T_{batch} \cup \{(h, \ell, t), (h', \ell, t')\}$ 
11:   end for
12:   Update embeddings w.r.t.
13: end loop
```

Entities and relations are initialized uniformly, and normalized

Negative sampling with triplet that does not appear in the KG

d represents distance
(negative of score)

$$\sum_{((h, \ell, t), (h', \ell, t')) \in T_{batch}} \nabla [\gamma + d(\mathbf{h} + \ell, \mathbf{t}) - d(\mathbf{h}' + \ell, \mathbf{t}')]_+$$

positive sample negative sample

Contrastive loss: favors lower distance (or higher score) for valid triplets, high distance (or lower score) for corrupted ones

Connectivity Patterns in KG

- Relations in a heterogeneous KG have different properties
 - Example:
 - Symmetry: If the edge $(h, \text{"Roommate"}, t)$ exists in KG, then the edge $(t, \text{"Roommate"}, h)$ should also exist.
 - Inverse relation: If the edge $(h, \text{"Advisor"}, t)$ exists in KG, then the edge $(t, \text{"Advisee"}, h)$ should also exist.
- Can we categorize these relation patterns?
- Are KG embedding methods (e.g., TransE) expressive enough to model these patterns?

Relation Patterns

- **Symmetric (Antisymmetric) Relations:**

$$r(h, t) \Rightarrow r(t, h) \quad (r(h, t) \Rightarrow \neg r(t, h)) \quad \forall h, t$$

- **Example:**

- Symmetric: Family, Roommate
 - Antisymmetric: Hyponym

- **Inverse Relations:**

$$r_2(h, t) \Rightarrow r_1(t, h)$$

- **Example :** (Advisor, Advisee)

- **Composition (Transitive) Relations:**

$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$

- **Example:** My mother's husband is my father.

- **1-to-N relations:**

- $r(h, t_1), r(h, t_2), \dots, r(h, t_n)$ are all True.

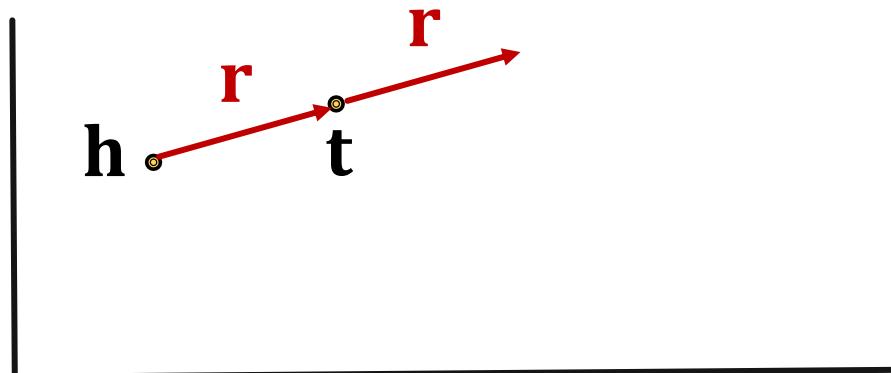
- **Example:** r is "StudentsOf"

Antisymmetric Relations in TransE

- **Antisymmetric Relations:**

$$r(h, t) \Rightarrow \neg r(t, h) \quad \forall h, t$$

- **Example:** Hyponym
- **TransE** can model antisymmetric relations ✓
- $\mathbf{h} + \mathbf{r} = \mathbf{t}$, but $\mathbf{t} + \mathbf{r} \neq \mathbf{h}$

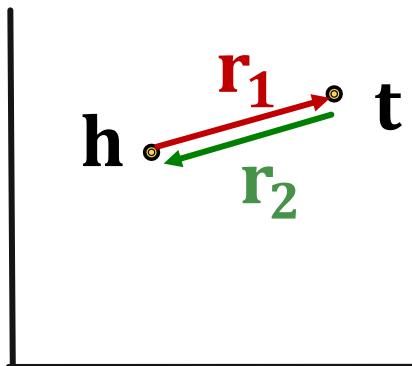


Inverse Relations in TransE

- Inverse Relations:

$$r_2(h, t) \Rightarrow r_1(t, h)$$

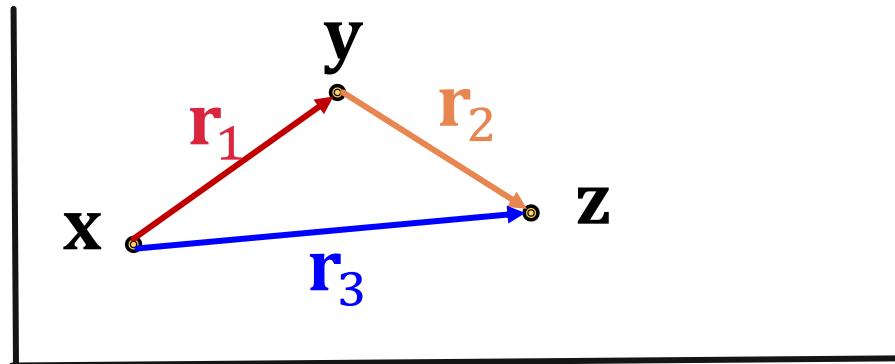
- Example : (Advisor, Advisee)
- TransE can model inverse relations ✓
- $h + r_2 = t$, we can set $r_1 = -r_2$



Composition in TransE

- **Composition (Transitive) Relations:**
$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$
- **Example:** My mother's husband is my father.
- **TransE** can model composition relations ✓

$$\mathbf{r}_3 = \mathbf{r}_1 + \mathbf{r}_2$$

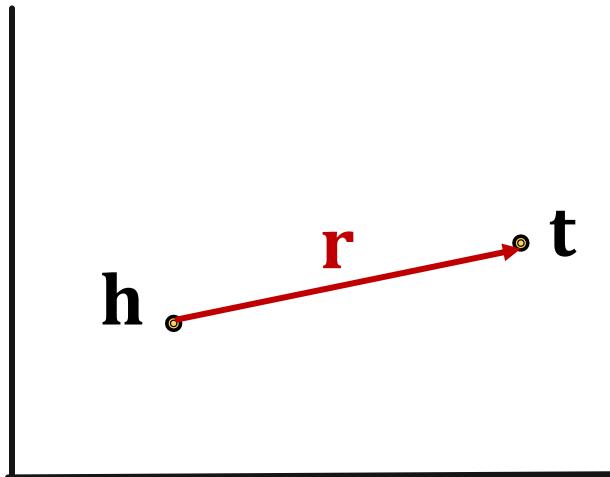


Limitation: Symmetric Relations

- **Symmetric Relations:**

$$r(h, t) \Rightarrow r(t, h) \quad \forall h, t$$

- **Example:** Family, Roommate
- **TransE cannot** model symmetric relations **x**
only if $\mathbf{r} = 0$, $\mathbf{h} = \mathbf{t}$

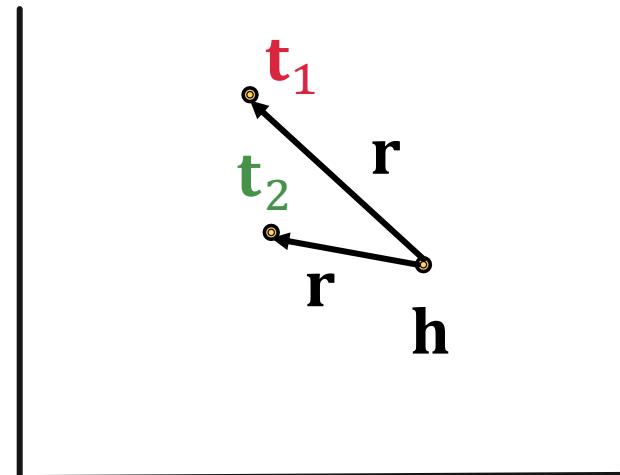


For all h, t that satisfy $r(h, t)$, $r(t, h)$ is also True, which means $\|\mathbf{h} + \mathbf{r} - \mathbf{t}\| = 0$ and $\|\mathbf{t} + \mathbf{r} - \mathbf{h}\| = 0$. Then $\mathbf{r} = 0$ and $\mathbf{h} = \mathbf{t}$, however h and t are two different entities and should be mapped to different locations.

Limitation: 1-to-N Relations

- **1-to-N Relations:**
 - **Example:** (h, r, t_1) and (h, r, t_2) both exist in the knowledge graph, e.g., r is “StudentsOf”
- **TransE cannot** model 1-to-N relations ✗
 - t_1 and t_2 will map to the same vector, although they are different entities

- $t_1 = h + r = t_2$
- $t_1 \neq t_2$ **contradictory!**



Stanford CS224W: Knowledge Graph Completion: TransR

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>

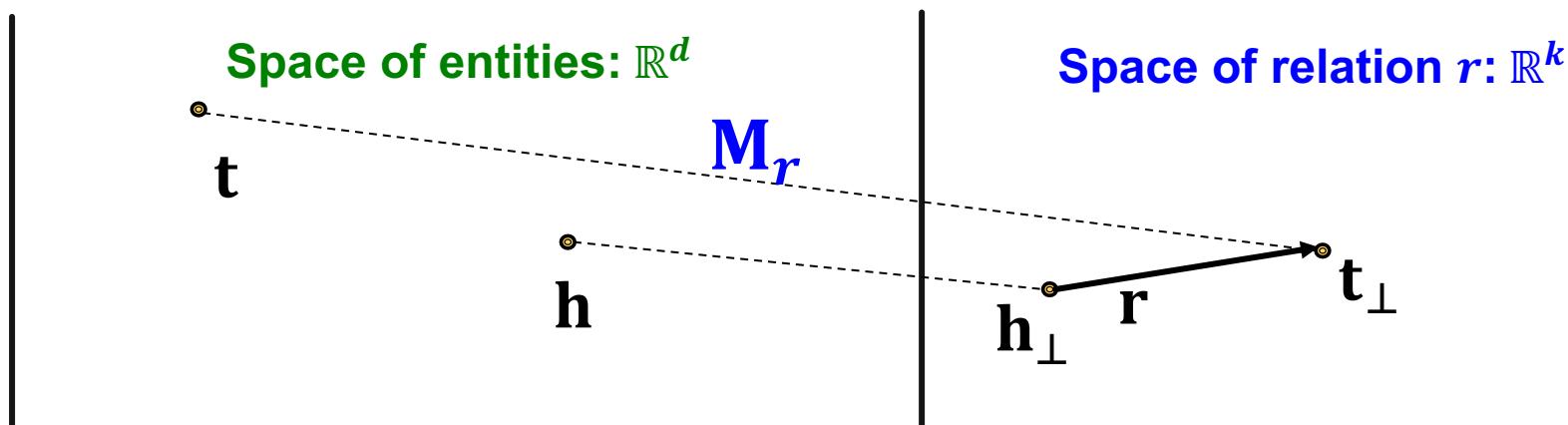


TransR

- TransE models translation of any relation in the **same** embedding space.
- Can we design a new space for each relation and do translation in **relation-specific space**?
- TransR: model **entities** as vectors in the entity space \mathbb{R}^d and model each **relation** as vector in relation space $\mathbf{r} \in \mathbb{R}^k$ with $\mathbf{M}_r \in \mathbb{R}^{k \times d}$ as the projection matrix.

TransR

- TransR: model **entities** as vectors in the entity space \mathbb{R}^d and model each **relation** as vector in relation space $\mathbf{r} \in \mathbb{R}^k$ with $\mathbf{M}_r \in \mathbb{R}^{k \times d}$ as the **projection matrix**.
Use \mathbf{M}_r to **project** from entity space \mathbb{R}^d to relation space \mathbb{R}^k !
- $\mathbf{h}_\perp = \mathbf{M}_r \mathbf{h}, \mathbf{t}_\perp = \mathbf{M}_r \mathbf{t}$
- **Score function:** $f_r(h, t) = -||\mathbf{h}_\perp + \mathbf{r} - \mathbf{t}_\perp||$



Symmetric Relations in TransR

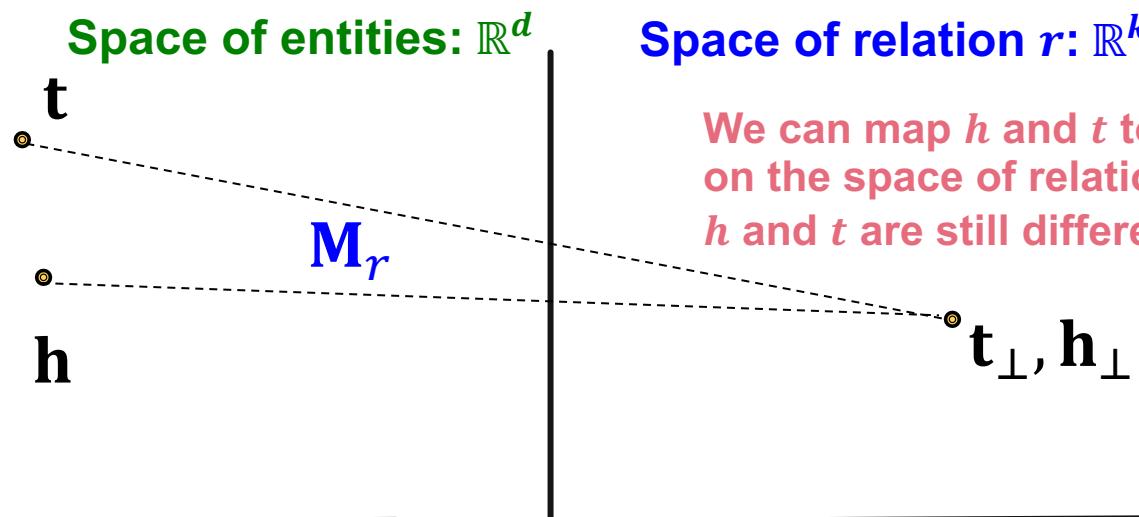
■ Symmetric Relations:

$$r(h, t) \Rightarrow r(t, h) \quad \forall h, t$$

- Example: Family, Roommate
- TransR can model symmetric relations

$$\mathbf{r} = 0, \quad \mathbf{h}_\perp = \mathbf{M}_r \mathbf{h} = \mathbf{M}_r \mathbf{t} = \mathbf{t}_\perp \checkmark$$

Note different
symmetric
relations may
have different \mathbf{M}_r



Antisymmetric Relations in TransR

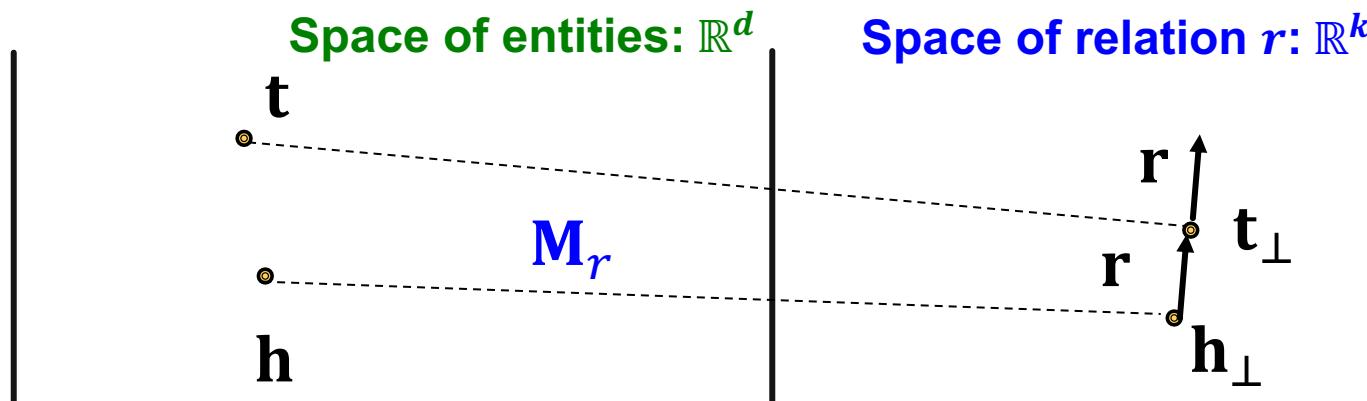
- **Antisymmetric Relations:**

$$r(h, t) \Rightarrow \neg r(t, h) \quad \forall h, t$$

- **Example:** Hyponym
- **TransR** can model antisymmetric relations

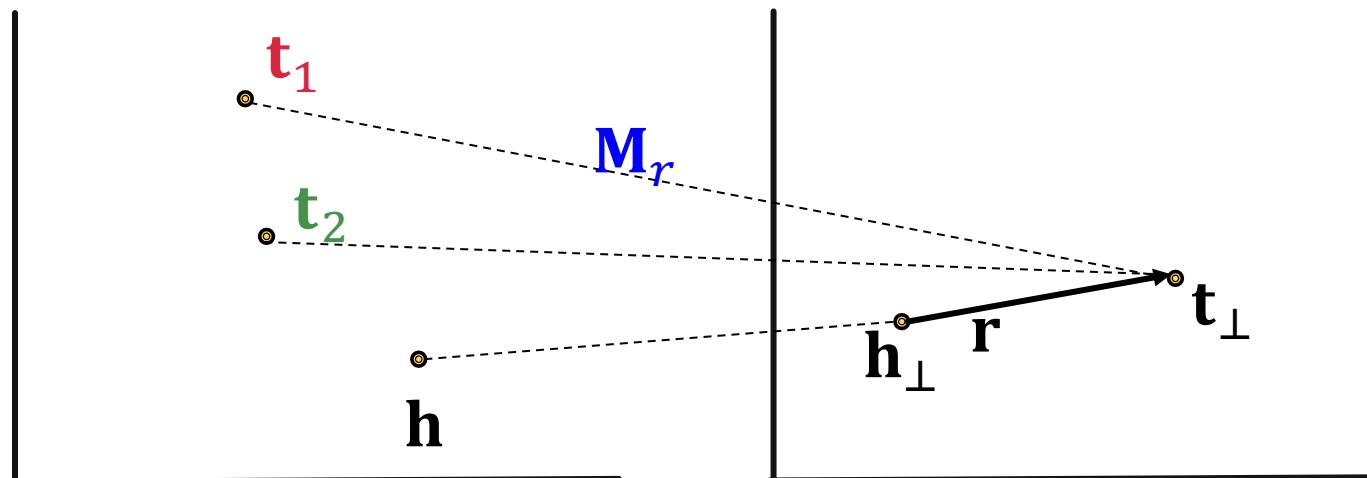
$$\mathbf{r} \neq 0, \mathbf{M}_r \mathbf{h} + \mathbf{r} = \mathbf{M}_r \mathbf{t},$$

Then $\mathbf{M}_r \mathbf{t} + \mathbf{r} \neq \mathbf{M}_r \mathbf{h}$ ✓



1-to-N Relations in TransR

- **1-to-N Relations:**
 - **Example:** If (h, r, t_1) and (h, r, t_2) exist in the knowledge graph.
- **TransR** can model 1-to-N relations ✓
 - We can learn \mathbf{M}_r so that $t_\perp = \mathbf{M}_r t_1 = \mathbf{M}_r t_2$
 - Note that t_1 does not need to be equal to t_2 !



Inverse Relations in TransR

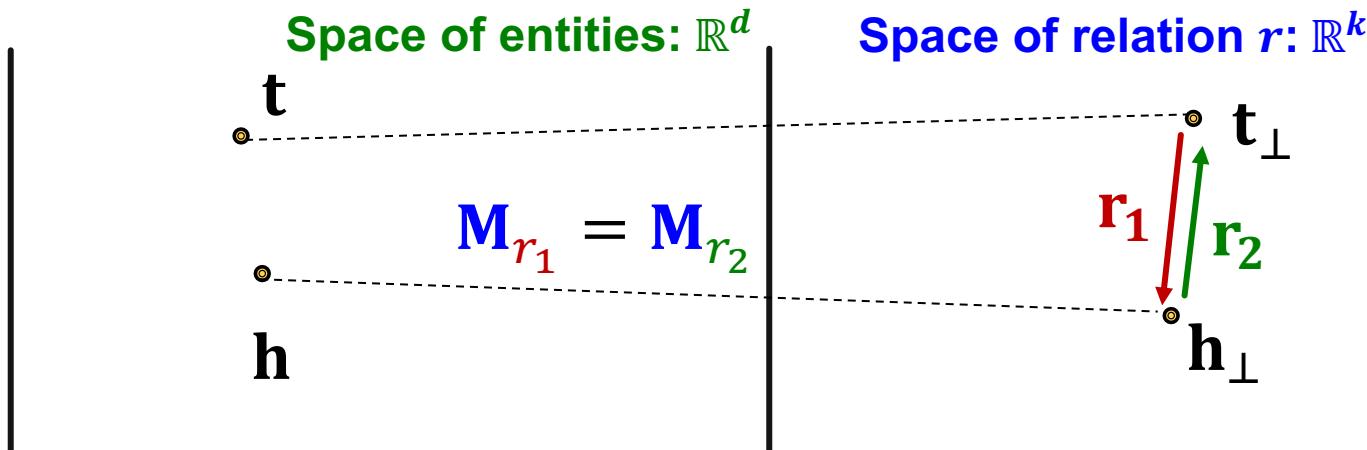
- Inverse Relations:

$$r_2(h, t) \Rightarrow r_1(t, h)$$

- Example : (Advisor, Advisee)
- TransR can model inverse relations

$$r_2 = -r_1, M_{r_1} = M_{r_2}$$

Then $M_{r_1}t + r_1 = M_{r_1}h$ and $M_{r_2}h + r_2 = M_{r_2}t$ ✓



Composition Relations in TransR

■ Composition Relations:

$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$

- Example: My mother's husband is my father.
- TransR ~~can~~ model composition relations

Cannot *Not naturally Compositional for multiple relations*

High-level intuition: TransR models a triple with linear functions, they are chainable.

Composition Relations in TransR

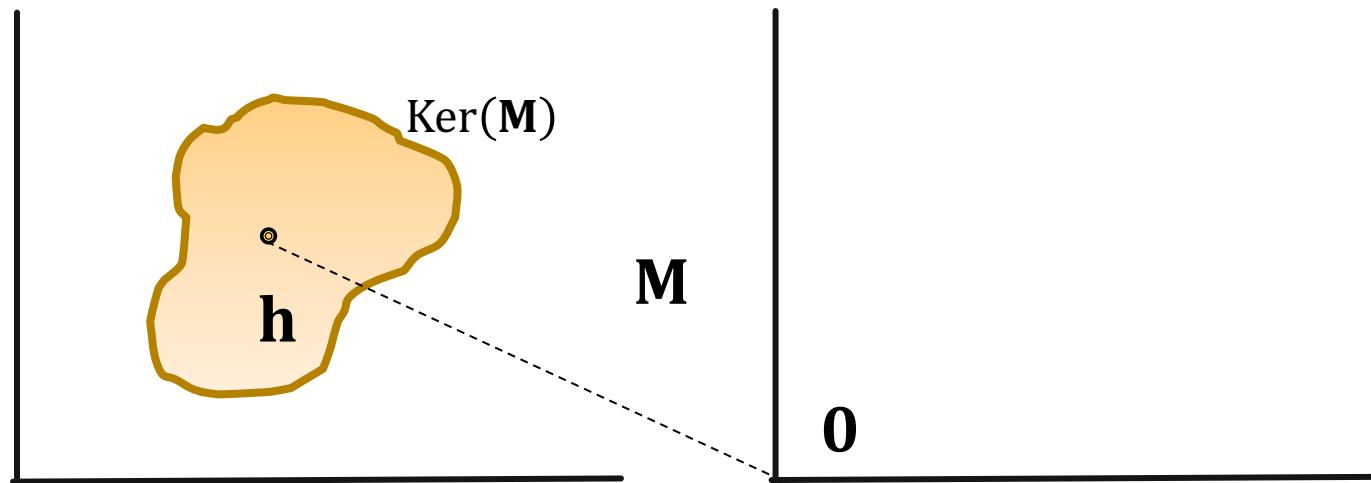
Composition Relations:

$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$

Background:

Kernel space of a matrix \mathbf{M} :

$$\mathbf{h} \in \text{Ker}(\mathbf{M}), \text{ then } \mathbf{M}\mathbf{h} = \mathbf{0}$$



Composition Relations in TransR

- **Composition Relations:**

$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$

Assume $\mathbf{M}_{r_1} \mathbf{g}_1 = \mathbf{r}_1$ and $\mathbf{M}_{r_2} \mathbf{g}_2 = \mathbf{r}_2$

- For $r_1(x, y)$:

$r_1(x, y)$ exists $\rightarrow \mathbf{M}_{r_1} \mathbf{x} + \mathbf{r}_1 = \mathbf{M}_{r_1} \mathbf{y} \rightarrow \mathbf{y} - \mathbf{x} \in \mathbf{g}_1 + \text{Ker}(\mathbf{M}_{r_1}) \rightarrow \mathbf{y} \in \mathbf{x} + \mathbf{g}_1 + \text{Ker}(\mathbf{M}_{r_1})$

- Same for $r_2(y, z)$:

$r_2(y, z)$ exists $\rightarrow \mathbf{M}_{r_2} \mathbf{y} + \mathbf{r}_2 = \mathbf{M}_{r_2} \mathbf{z} \rightarrow \mathbf{z} - \mathbf{y} \in \mathbf{g}_2 + \text{Ker}(\mathbf{M}_{r_2}) \rightarrow \mathbf{z} \in \mathbf{y} + \mathbf{g}_2 + \text{Ker}(\mathbf{M}_{r_2})$

- Then,

We have $\mathbf{z} \in \mathbf{x} + \mathbf{g}_1 + \mathbf{g}_2 + \text{Ker}(\mathbf{M}_{r_1}) + \text{Ker}(\mathbf{M}_{r_2})$

Composition Relations in TransR

- **Composition Relations:**

$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$

We have $\mathbf{z} \in \mathbf{x} + \mathbf{g}_1 + \mathbf{g}_2 + \text{Ker}(\mathbf{M}_{r_1}) + \text{Ker}(\mathbf{M}_{r_2})$

- Construct \mathbf{M}_{r_3} , s.t. $\text{Ker}(\mathbf{M}_{r_3}) = \text{Ker}(\mathbf{M}_{r_1}) + \text{Ker}(\mathbf{M}_{r_2})$
- Since

- $\dim(\text{Ker}(\mathbf{M}_{r_3})) \geq \dim(\text{Ker}(\mathbf{M}_{r_1}))$
- \mathbf{M}_{r_3} has the same shape as \mathbf{M}_{r_1}

We know \mathbf{M}_{r_3} exists!

- Set $\mathbf{r}_3 = \mathbf{M}_{r_3}(\mathbf{g}_1 + \mathbf{g}_2)$
- We are done! We have $\mathbf{M}_{r_3}\mathbf{x} + \mathbf{r}_3 = \mathbf{M}_{r_3}\mathbf{z}$

Stanford CS224W: Knowledge Graph Completion: DistMult

CS224W: Machine Learning with Graphs

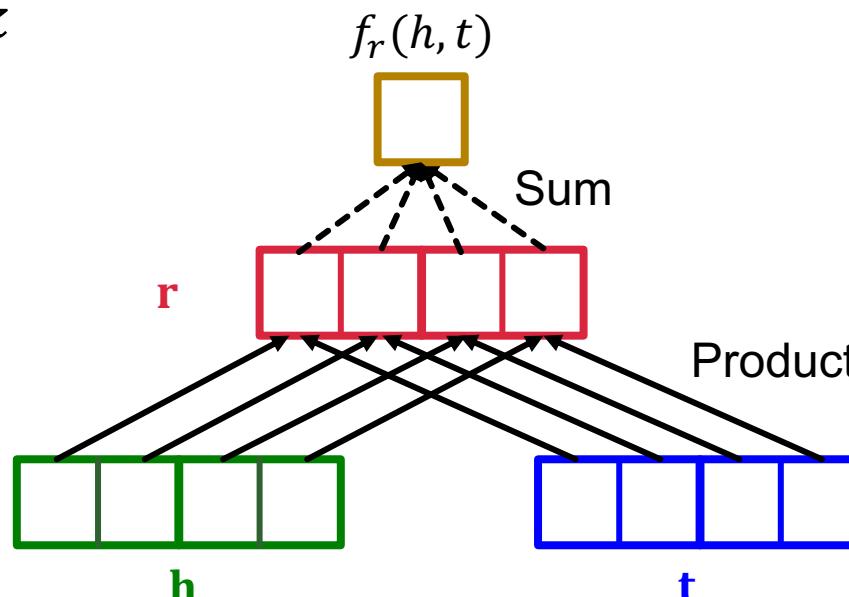
Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



New Idea: Bilinear Modeling

- So far: The scoring function $f_r(h, t)$ is **negative of L1 / L2 distance** in **TransE** and **TransR**
- Another line of KG embeddings adopt **bilinear** modeling
- **DistMult**: Entities and relations using vectors in \mathbb{R}^k
- **Score function:** $f_r(h, t) = \langle \mathbf{h}, \mathbf{r}, \mathbf{t} \rangle = \sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \mathbf{t}_i$
- $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^k$

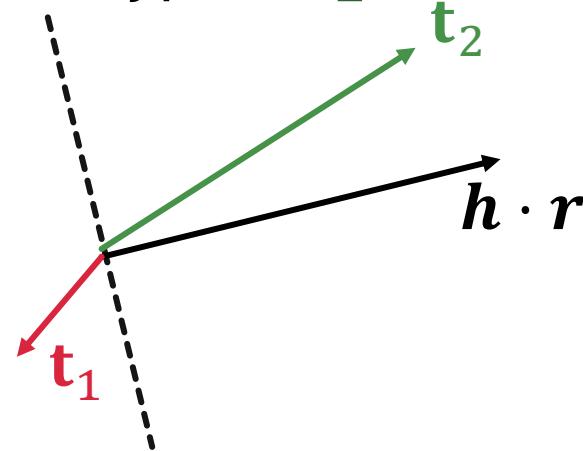


DistMult

Hyper plane

- **DistMult**: Entities and relations using vectors in \mathbb{R}^k
- **Score function**: $f_r(h, t) = \langle h, r, t \rangle = \sum_i h_i \cdot r_i \cdot t_i$
 - $h, r, t \in \mathbb{R}^k$
- **Intuition of the score function**: Can be viewed as a **cosine similarity** between $h \cdot r$ and t
 - where $h \cdot r$ is defined as $\sum_i h_i \cdot r_i$
- **Example**:

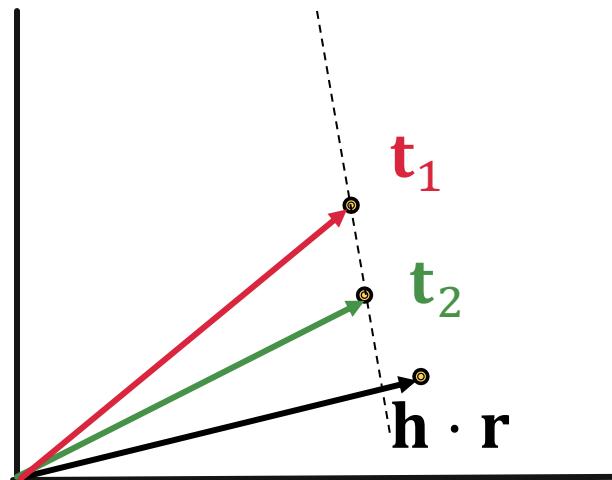
$$f_r(h, t_1) < 0, \quad f_r(h, t_2) > 0$$



1-to-N Relations in DistMult

- **1-to-N Relations:**
 - **Example:** If (h, r, t_1) and (h, r, t_2) exist in the knowledge graph
- **Distmult** can model 1-to-N relations ✓

$$\langle h, r, t_1 \rangle = \langle h, r, t_2 \rangle$$



Symmetric Relations in DistMult

- **Symmetric Relations:**

$$r(h, t) \Rightarrow r(t, h) \quad \forall h, t$$

- **Example:** Family, Roommate
- **DistMult** can naturally model symmetric relations ✓

$$\begin{aligned} f_r(h, t) = < \mathbf{h}, \mathbf{r}, \mathbf{t} > &= \sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \mathbf{t}_i = \\ &< \mathbf{t}, \mathbf{r}, \mathbf{h} > = f_r(t, h) \end{aligned}$$

Limitation: Antisymmetric Relations

- **Antisymmetric Relations:**

$$r(h, t) \Rightarrow \neg r(t, h) \quad \forall h, t$$

- **Example:** Hypernym
- **DistMult cannot** model antisymmetric relations

$$f_r(h, t) = \langle h, r, t \rangle = \langle t, r, h \rangle = f_r(t, h) \times$$

- $r(h, t)$ and $r(t, h)$ always have same score!

Limitation: Inverse Relations

- **Inverse Relations:**

$$r_2(h, t) \Rightarrow r_1(t, h)$$

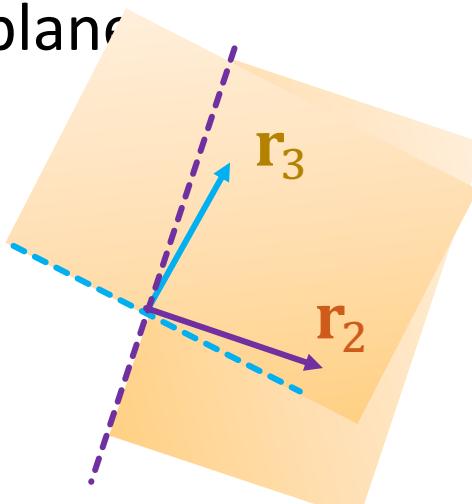
- **Example :** (Advisor, Advisee)
- **DistMult cannot** model inverse relations ✗
 - If it does model inverse relations:
 $f_{r_2}(h, t) = \langle \mathbf{h}, \mathbf{r}_2, \mathbf{t} \rangle = \langle \mathbf{t}, \mathbf{r}_1, \mathbf{h} \rangle = f_{r_1}(t, h)$
 - This means $\mathbf{r}_2 = \mathbf{r}_1$
 - But semantically this does not make sense: **The embedding of “Advisor” should not be the same with “Advisee”.**

Limitation: Composition Relations

- **Composition Relations:**

$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$

- **Example:** My mother's husband is my father.
- **DistMult cannot** model composition relations ✗
- **Intuition:** **DistMult** defines a hyperplane for each (head, relation), the union of the hyperplane induced by multi-hops of relations, e.g., (r_1, r_2) , cannot be expressed using a single hyperplane



Stanford CS224W: Knowledge Graph Completion: ComplEx

CS224W: Machine Learning with Graphs

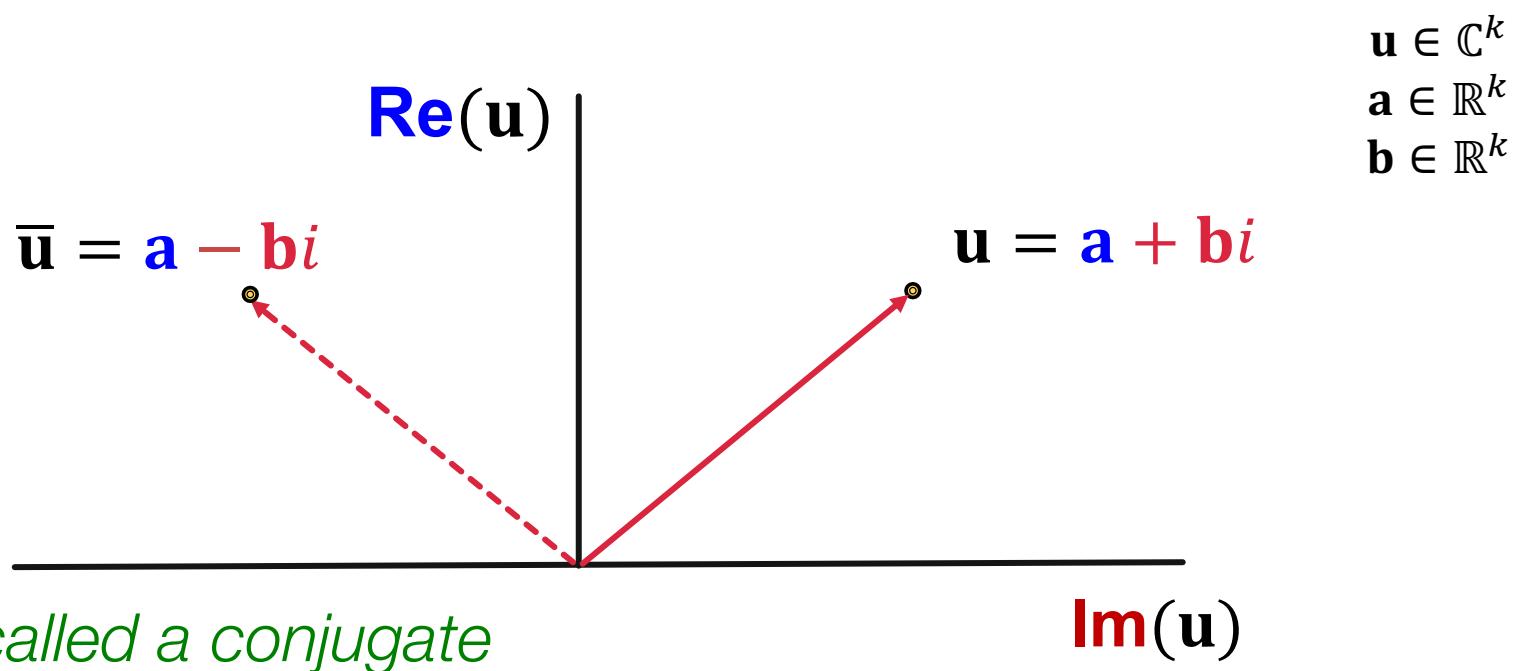
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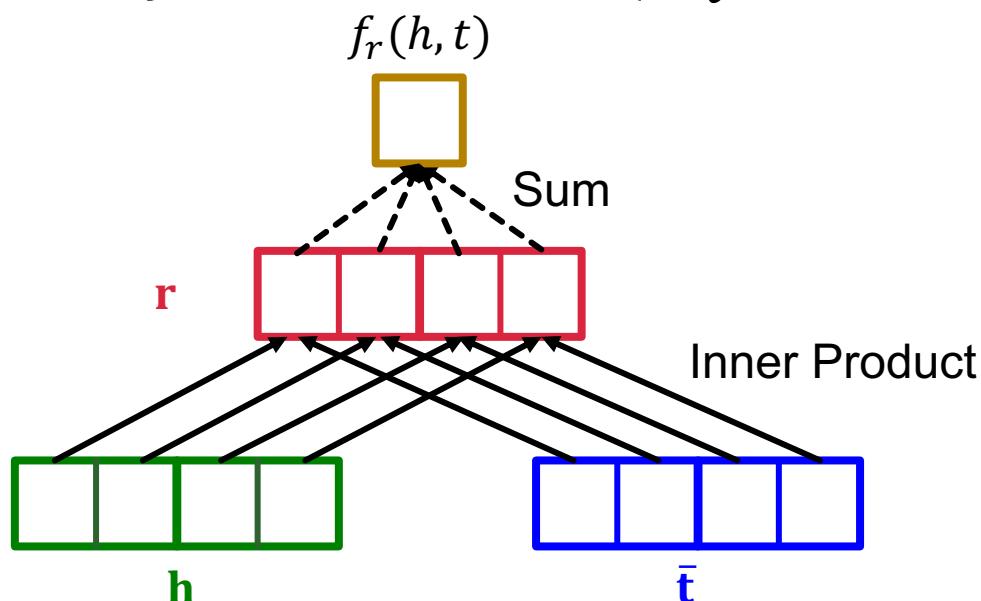
ComplEx

- Based on Distmult, ComplEx embeds entities and relations in **Complex vector space**
- ComplEx: model entities and relations using vectors in \mathbb{C}^k



ComplEx

- Based on Distmult, ComplEx embeds entities and relations in **Complex vector space**
- ComplEx: model entities and relations using vectors in \mathbb{C}^k
- **Score function** $f_r(h, t) = \text{Re}(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i)$



Antisymmetric Relations in ComplEx

- **Antisymmetric Relations:**

$$r(h, t) \Rightarrow \neg r(t, h) \quad \forall h, t$$

- **Example:** Hyponym
- **ComplEx** can model antisymmetric relations ✓
 - The model is expressive enough to learn
 - **High** $f_r(h, t) = \text{Re}(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i)$
 - **Low** $f_r(t, r) = \text{Re}(\sum_i \mathbf{t}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{h}}_i)$

Due to the asymmetric modeling using complex conjugate.

Symmetric Relations in ComplEx

- **Symmetric Relations:**

$$r(h, t) \Rightarrow r(t, h) \quad \forall h, t$$

- **Example:** Family, Roommate
- **ComplEx** can model symmetric relations ✓

- When $\text{Im}(\mathbf{r}) = 0$, we have

$$\begin{aligned} f_r(h, t) &= \text{Re}(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i) = \sum_i \text{Re}(\mathbf{r}_i \cdot \mathbf{h}_i \cdot \bar{\mathbf{t}}_i) \\ &= \sum_i \mathbf{r}_i \cdot \text{Re}(\mathbf{h}_i \cdot \bar{\mathbf{t}}_i) = \sum_i \mathbf{r}_i \cdot \text{Re}(\bar{\mathbf{h}}_i \cdot \mathbf{t}_i) = \sum_i \text{Re}(\mathbf{r}_i \cdot \bar{\mathbf{h}}_i \cdot \mathbf{t}_i) \\ &= f_r(t, h) \end{aligned}$$

Inverse Relations in ComplEx

- Inverse Relations:

$$r_2(h, t) \Rightarrow r_1(t, h)$$

- Example : (Advisor, Advisee)
- ComplEx can model inverse relations ✓
 - $r_1 = \bar{r}_2$
 - Complex conjugate of
 $r_2 = \underset{\mathbf{r}}{\operatorname{argmax}} \operatorname{Re}(\langle \mathbf{h}, \mathbf{r}, \bar{\mathbf{t}} \rangle)$ is exactly
 $r_1 = \underset{\mathbf{r}}{\operatorname{argmax}} \operatorname{Re}(\langle \mathbf{t}, \mathbf{r}, \bar{\mathbf{h}} \rangle).$

Composition and 1-to-N

■ Composition Relations:

$$r_1(x, y) \wedge r_2(y, z) \Rightarrow r_3(x, z) \quad \forall x, y, z$$

- Example: My mother's husband is my father.

■ 1-to-N Relations:

- Example: If (h, r, t_1) and (h, r, t_2) exist in the knowledge graph
- ComplEx share the same property with DistMult
 - Cannot model composition relations
 - Can model 1-to-N relations

Expressiveness of All Models

- Properties and expressive power of different KG completion methods:

Model	Score	Embedding	Sym.	Antisym.	Inv.	Compos.	1-to-N
TransE	$-\ \mathbf{h} + \mathbf{r} - \mathbf{t}\ $	$\mathbf{h}, \mathbf{t}, \mathbf{r} \in \mathbb{R}^k$	✗	✓	✓	✓	✗
TransR	$-\ M_r \mathbf{h} + \mathbf{r} - M_r \mathbf{t}\ $	$\mathbf{h}, \mathbf{t}, \mathbf{r} \in \mathbb{R}^k, M_r \in \mathbb{R}^{d \times k}$	✓	✓	✓	✗	✓
DistMult	$\langle \mathbf{h}, \mathbf{r}, \mathbf{t} \rangle$	$\mathbf{h}, \mathbf{t}, \mathbf{r} \in \mathbb{R}^k$	✓	✗	✗	✗	✓
ComplEx	$\text{Re}(\langle \mathbf{h}, \mathbf{r}, \bar{\mathbf{t}} \rangle)$	$\mathbf{h}, \mathbf{t}, \mathbf{r} \in \mathbb{C}^k$	✓	✓	✓	✗	✓

KG Embeddings in Practice

1. Different KGs may have **drastically different relation patterns!**
2. There is not a general embedding that works for all KGs, use the **table** to select models
3. Try **TransE** for a quick run if the target KG does not have much symmetric relations
4. Then use more expressive models, e.g.,
ComplEx, **RotatE** (**TransE** in Complex space)

Summary of the second part

- Link prediction / Graph completion is one of the prominent tasks on knowledge graphs
- Introduce **TransE** / **TransR** / **DistMult** / **ComplEx** models with different embedding space and expressiveness

TransE Training

I like this slide.
Let's include it!
And discuss this topic a
bit more.

- Translation Intuition: for a triple $(h,$

$$\mathbf{h} + \mathbf{r} = \mathbf{t}$$

Max margin loss:

$$\mathcal{L} = \sum_{(h,r,t) \in G, (h,r,t') \notin G} [\gamma + f_r(h, t) - f_r(h, t')]_+$$

Valid triple Corrupted triple

where γ is the margin, i.e., the smallest distance tolerated by the model between a valid triple and a corrupted one.

NOTE: check
lecture 7 for a more
in-depth discussion
of TransE!