Yale

Knowledge Graph Embeddings

CPSC483: Deep Learning on Graph-Structured Data

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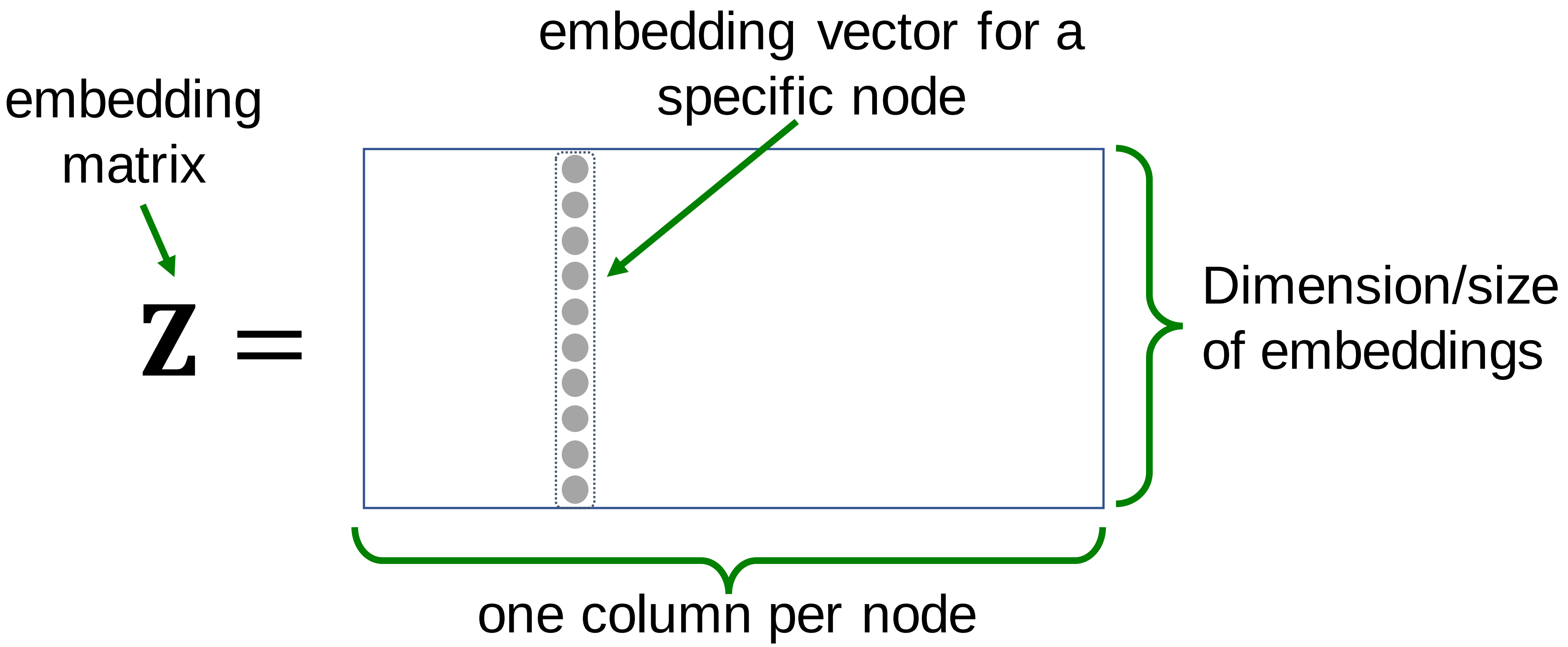
Readings

- Readings are updated on the website (syllabus page)
- **Lecture 18 readings:**
  - Node2Vec
  - Graph Representation Learning survey
- **Lecture 19 readings:**
  - TransE: Translating Embeddings for Modeling Multi-relational Data
  - RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space
  - TuckER: Tensor Factorization for Knowledge Graph Completion

Recap: Distributed Node Embeddings (1)

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



Recap: Distributed Node Embeddings (2)

An **unsupervised** setting for learning node embeddings

1. **Encoder ENC** maps from nodes to embeddings
2. **Define a node similarity function** (i.e., a measure of similarity in the original network)
3. **Decoder DEC** maps from embeddings to the similarity score
4. **Optimize the parameters of the encoder so that:**

$$\text{similarity}(u, v) \approx \mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$$

Today: we define other **objectives** to learn node embeddings

Content

- **Introduction: Knowledge Graph**

- **Knowledge Graph Embedding Models**
  - **TransE**
  - **DistMult & ComplEx**
  - **RotatE**
  - **TuckER**

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- **Introduction: Knowledge Graph**

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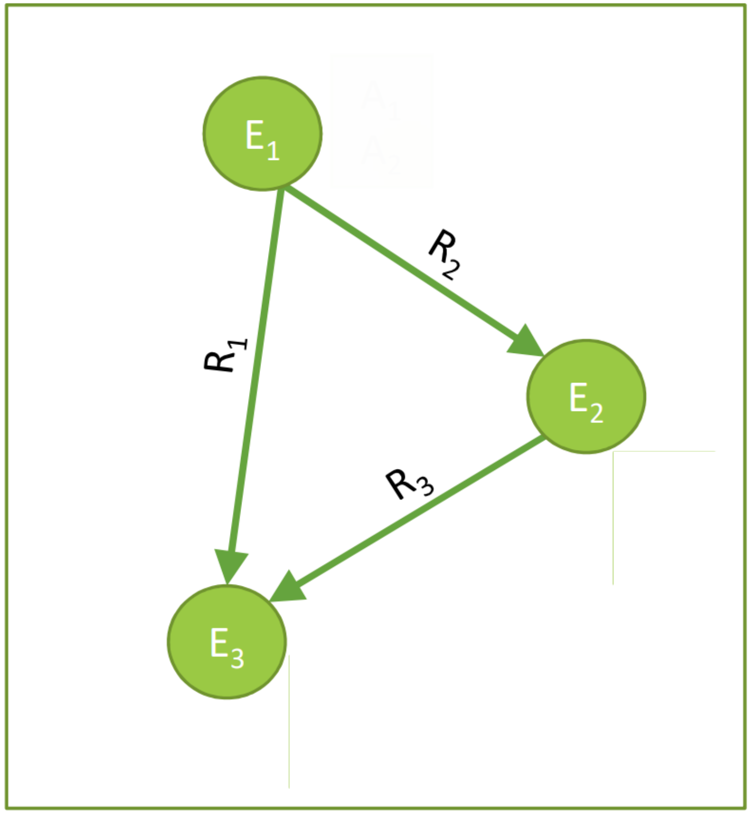
Knowledge Graphs (KG)

Knowledge as a graph:

- A set of triplets <head entity, relationship, tail entity>
- Capture entities, types, and relationships

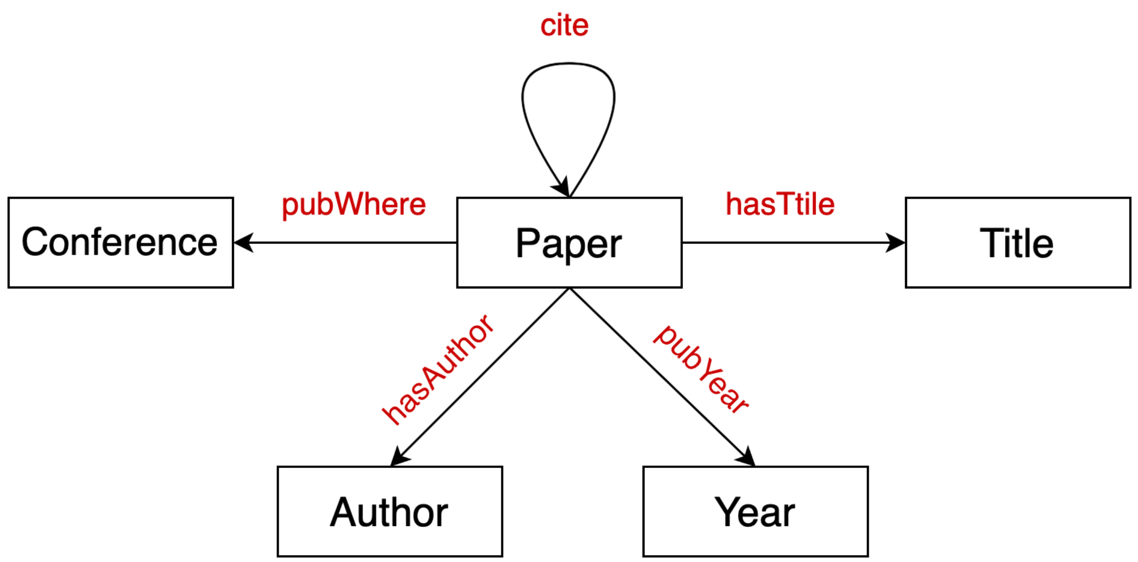
- Nodes are **entities**
- Nodes are labeled with their **types**
- Edges between two nodes capture **relationships** between entities
- **KG is an example of a heterogeneous graph**
  - **Recap:** Heterogenous graph is a graph with multiple node types and edge types



E: entity
R: relation

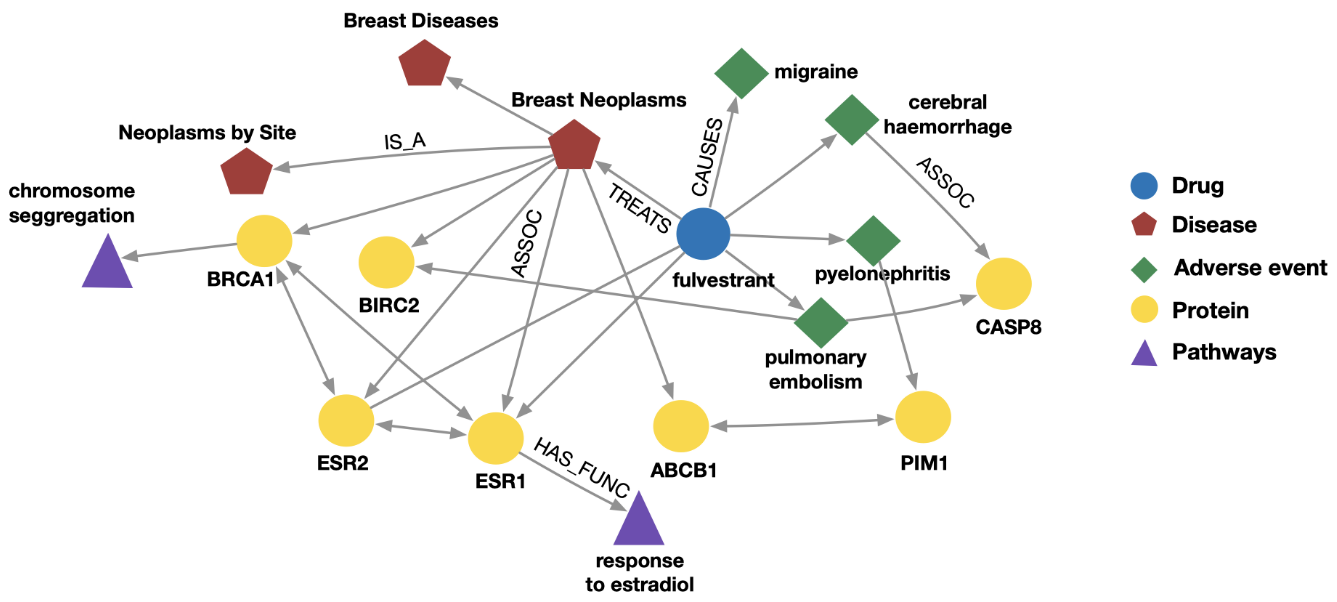
Example: Bibliographic Networks

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



Example: Biomedical 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 (Knowledge Vault)
- Amazon Product Graph
- Facebook Graph API
- Project Hanover/Literome
- LinkedIn Knowledge Graph
- Yandex Object Answer
- NELL (Never Ending Language Learning)

Applications of Knowledge Graphs

- **Serving information**

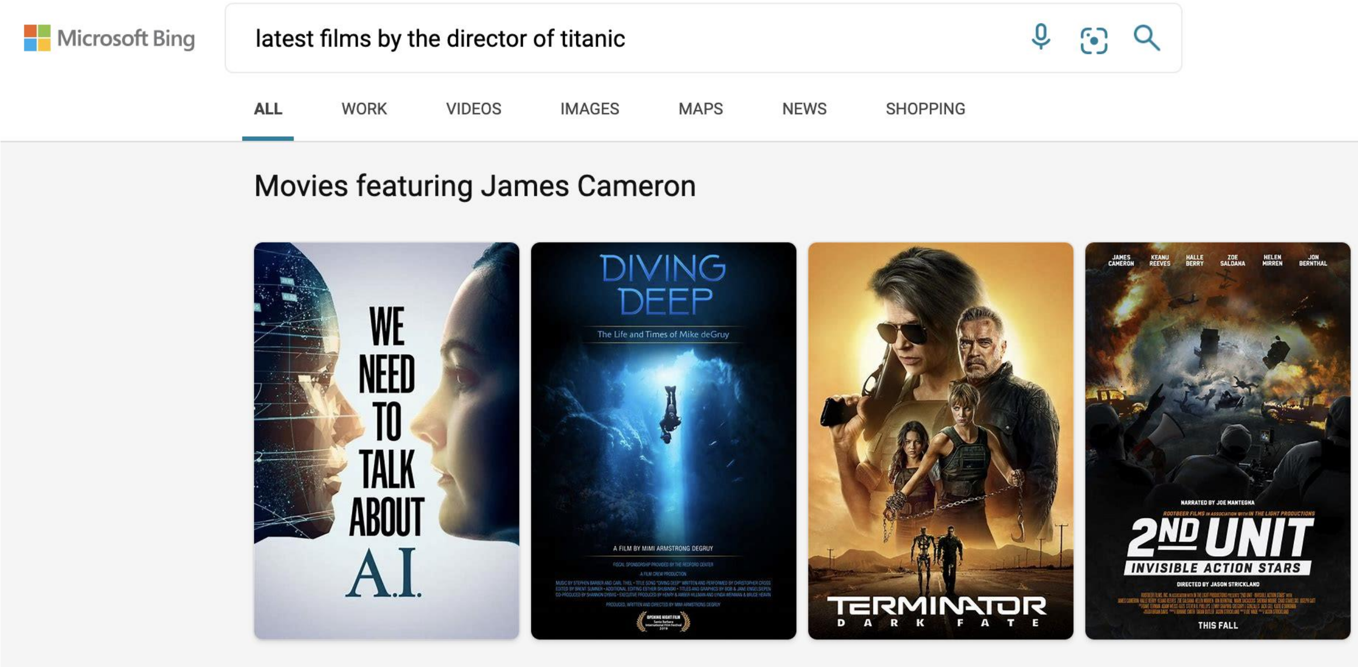


Image credit: Bing

Applications of Knowledge Graphs

- **Question answering and conversation agents**

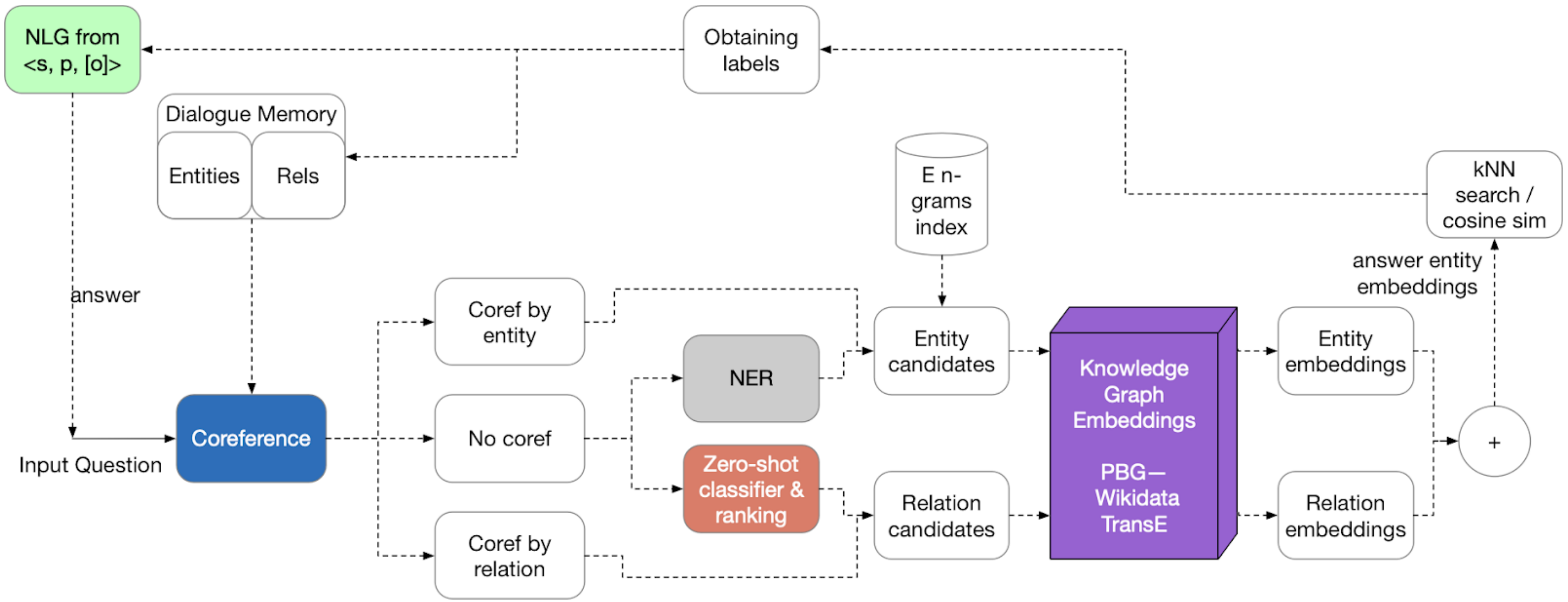


Image credit: Medium

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**
  - ~50 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.

KG Completion Task

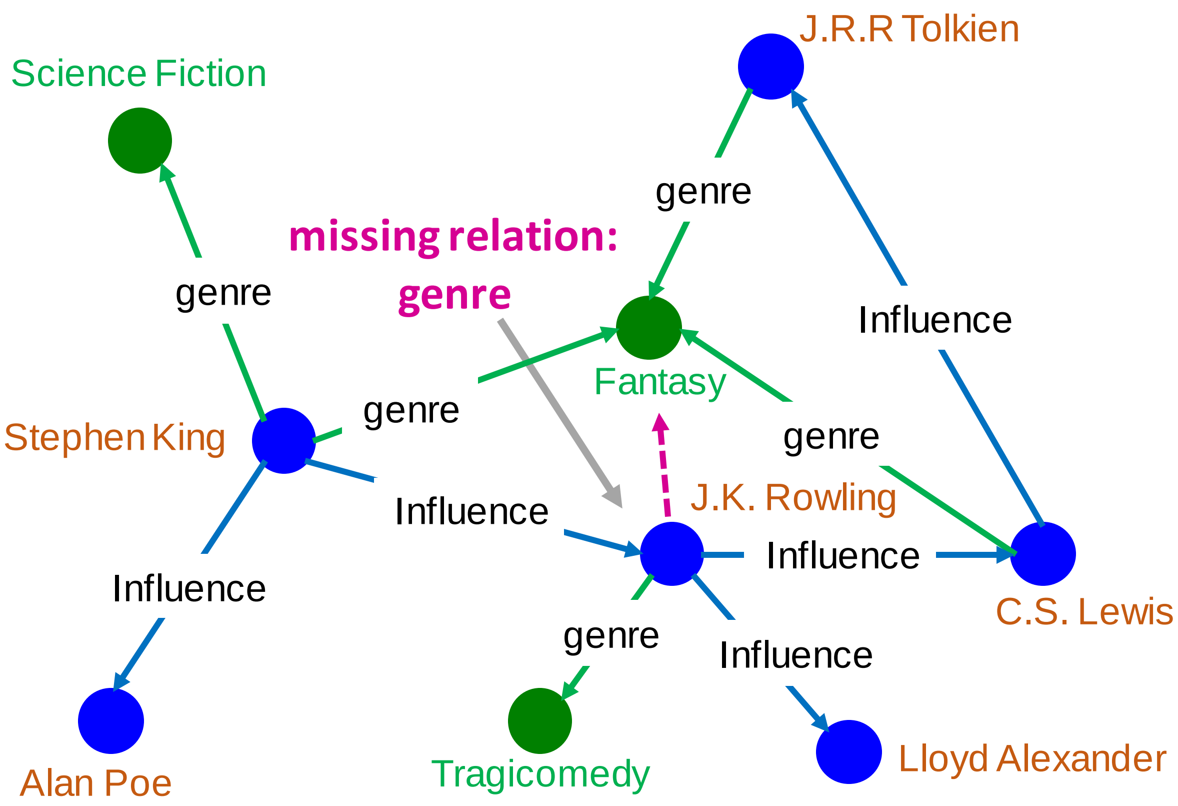
Knowledge graphs are usually incomplete. Many facts are missing!

Given an enormous KG, how can we complete the KG?

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

Recap: In link prediction task, we predict the edge $e = (u, v)$ based on the embeddings of head node u and tail node v

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



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**
    - **Deep encoder (GNN) is also possible here, using the same loss**
  - 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?

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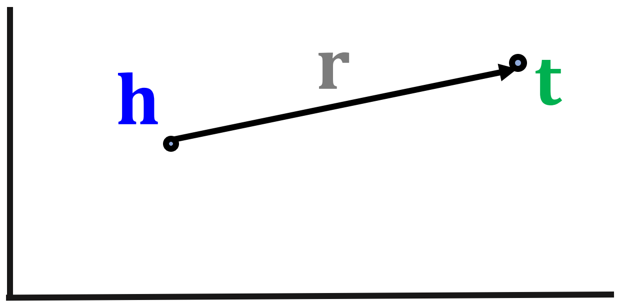
Translating Embeddings: TransE

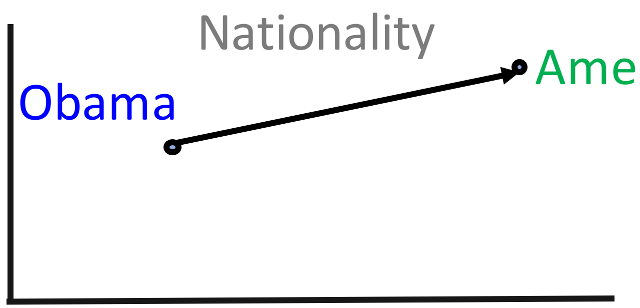
- **Translation Intuition**:

  For a triple (h, r, t), $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^k$ are the embedding vectors
  $\mathbf{h} + \mathbf{r} \approx \mathbf{t}$ if the given fact is true
  else $\mathbf{h} + \mathbf{r} \neq \mathbf{t}$

embedding vectors will appear in boldface

- **Scoring function**: $f_r(h, t) = -||\mathbf{h} + \mathbf{r} - \mathbf{t}||$
- Scoring function is **maximized** if the fact is **true**!





Bordes, et al., Translating embeddings for modeling multi-relational data, NeurIPS 2013.

Embedding Initialization

- Entities and relations are **initialized uniformly and then normalized**
- Given Training set $S = \{(h, r, t)\}$, where $h, t \in E, r \in R$.
  (**entity set E**, **relation set R**, **embedding dimension k**)
- For each r in the relation set R,
  - initialize $r \sim \text{uniform}(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$ → Xavier Initialization (see more details in original paper)
  - $r = r/\|r\|$ → Normailization
- For each e in the entity set E,
  - initialize $e \sim \text{uniform}(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$
  - $e = e/\|e\|$

Negative Sampling

- **Negative sampling** with triplet that does not appear in the KG
- Set of **corrupted triplets**:

$$S'_{(h,l,t)} = \{(h', r, t) | h' \in E\} \cup \{(h, r, t') | t' \in E\}$$

replace either the head or tail entity by a random entity in entity set E (but not both at the same time) in training triplets

What will happen if no negative examples are provided?

TransE Training

- Translation Intuition: for a triple (h, r, t),

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

Max margin loss:

0 if the term is negative

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

Valid triple

Corrupted triple (negative example)

corrupted set of (h, r, t)

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

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:**

$$\textbf{Symmetric: } r(h,t) \Rightarrow r(t,h) \;\; (\textbf{Antisymmetric: } r(h,t) \Rightarrow \neg r(t,h)) \quad \forall h,t$$

  - **Example**:
    - Symmetric: Family, Roommate
- **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:**

$$r(h,t_1), r(h,t_2), \dots, r(h,t_n) \text{ are all True.}$$

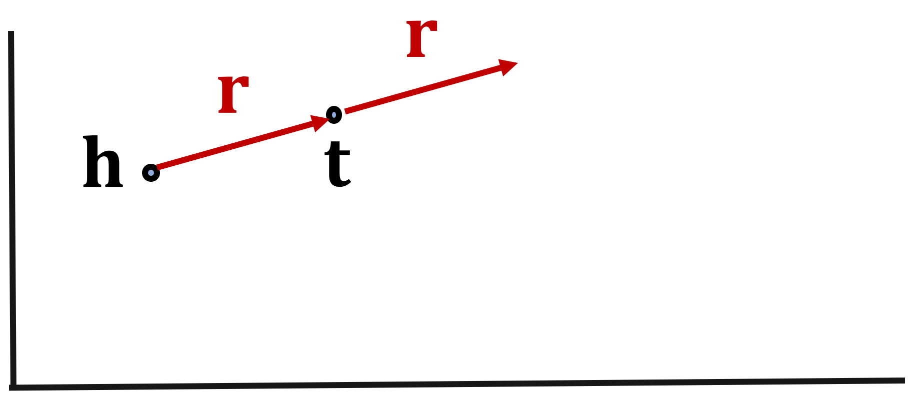
  - **Example**: r is "StudentsOf"

Antisymmetric Relations in TransE

- **Antisymmetric Relations:**

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

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

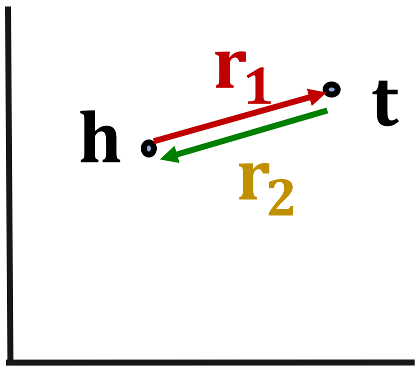


Inverse Relations in TransE

- **Inverse Relations:**

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

  - **Example** : (Advisor, Advisee)
- **TransE** can model inverse relations ✓
  - $\mathbf{h} + \mathbf{r}_2 = \mathbf{t}$, we can set $\mathbf{r}_1 = -\mathbf{r}_2$



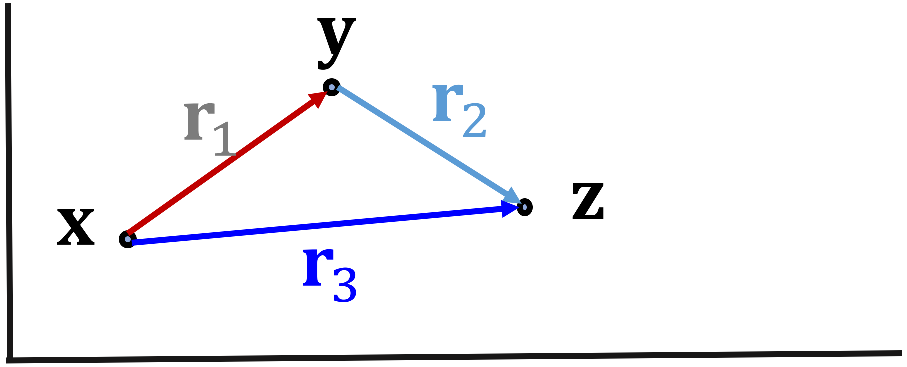
Composition in TransE

- **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.
- **TransE** can model composition relations✓

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

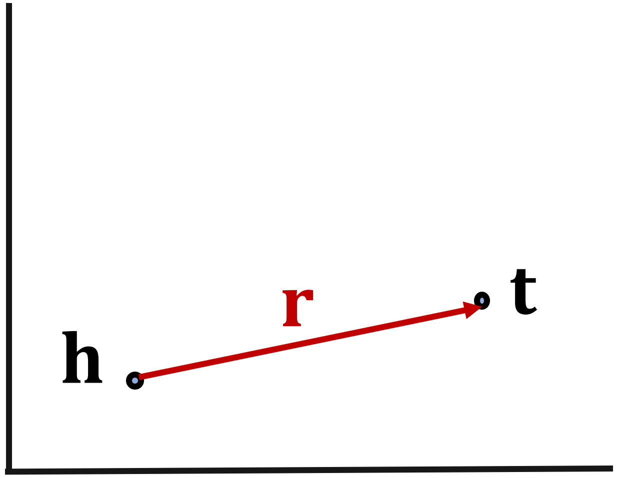


Limitation: Symmetric Relations

- **Symmetric Relations:**

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

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



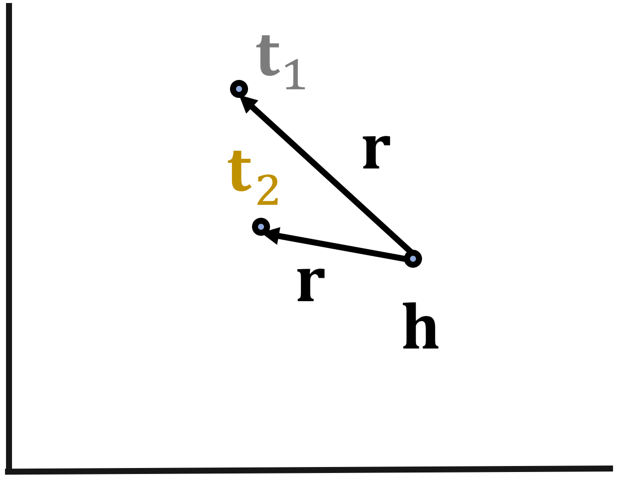
For all h, t that satisfy $r(h,t)$, $r(t,h)$ is also True, which means $||\mathbf{h} + \mathbf{r} - \mathbf{t}|| = 0$ and $||\mathbf{t} + \mathbf{r} - \mathbf{h}|| = 0$. Then $\mathbf{r} = 0$ and $\mathbf{h} = \mathbf{t}$, however h and t are two different entities and should be mapped to different locations.

Limitation: 1-to-N Relations

- **1-to-N Relations:**
  - (h, r, t_1) and (h, r, t_2) both exist in the knowledge graph
  - **Example**: r is "StudentsOf"
- **TransE cannot** model 1-to-N relations ✘
  - $\mathbf{t}_1$ and $\mathbf{t}_2$ will map to the same vector, although they are different entities

  - $\mathbf{t}_1 = \mathbf{h} + \mathbf{r} = \mathbf{t}_2$
  - $\mathbf{t}_1 \neq \mathbf{t}_2$

contradictory!



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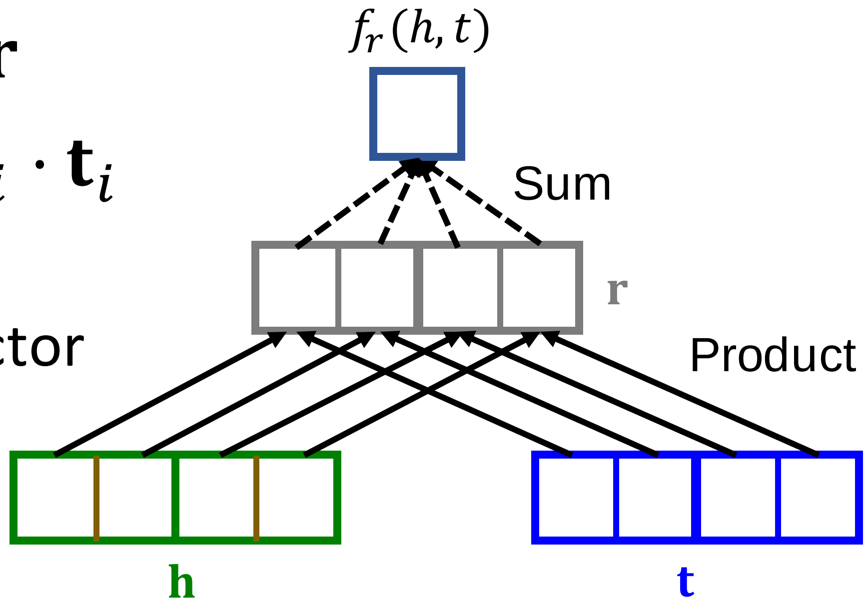
New Idea: Bilinear Modeling

- **So far:** The scoring function $f_r(h,t)$ is the **negative L2 distance**
- **DistMult** considers **bilinear** modeling
- Entities are embedded as vectors in $\mathbb{R}^k$
- **Score function**: $f_r(h,t) = \mathbf{h}^{\mathrm{T}}\, M_{\mathbf{r}}\mathbf{t}$
  - $M_{\mathbf{r}}$ is a learnable matrix parameter for relation $\mathbf{r}$
- A simpler version: $f_r(h,t) =< \mathbf{h}, \mathbf{r}, \mathbf{t} > = \sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \mathbf{t}_i$
  - Let $M_{\mathbf{r}}$ be a diagonal matrix
  - $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^k$ and i denotes the i-th dimension in the vector

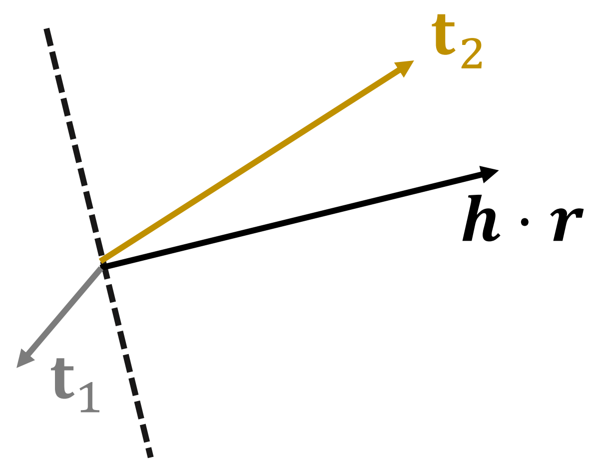


Yang et al, Embedding Entities and Relations for Learning and Inference in Knowledge Bases, ICLR 2015

DistMult

- **DistMult**: Entities and relations using vectors in $\mathbb{R}^k$
- **Score function:** $f_r(h,t) =< \mathbf{h}, \mathbf{r}, \mathbf{t} > = \sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \mathbf{t}_i$; $\quad \mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^k$
- **Intuition of the score function:** Can be viewed as a **cosine similarity** between $\mathbf{h} \cdot \mathbf{r}$ and $\mathbf{t}$
- **Example:**

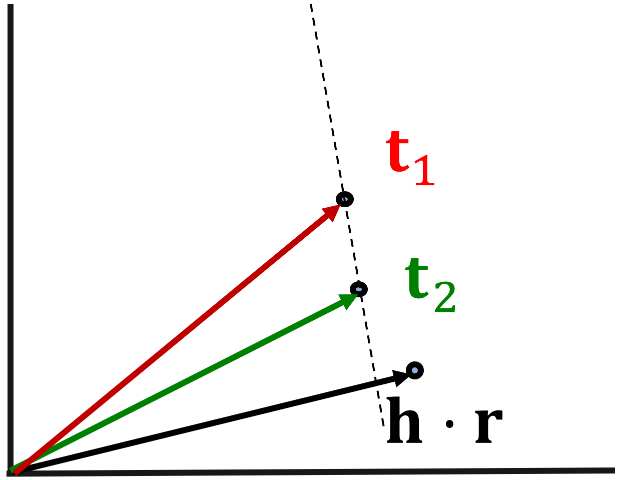
$$f_r(h, t_1) < 0, \qquad f_r(h, t_2) > 0$$



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 ✓

$$< \mathbf{h}, \mathbf{r}, \mathbf{t}_1 > = < \mathbf{h}, \mathbf{r}, \mathbf{t}_2 >$$



The projection of $\mathbf{t}_1$ and $\mathbf{t}_2$ along the vector $\mathbf{h} \cdot \mathbf{r}$ is the same

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

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

$$<\mathbf{t},\mathbf{r},\mathbf{h}> = f_r(t,h) \checkmark$$

Limitation: Antisymmetric Relations

- **Antisymmetric Relations:**

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

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

$$f_r(h,t) =< \mathbf{h}, \mathbf{r}, \mathbf{t} > = < \mathbf{t}, \mathbf{r}, \mathbf{h} >= f_r(t,h) \text{ ✘}$$

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

Limitation: Composition Relations

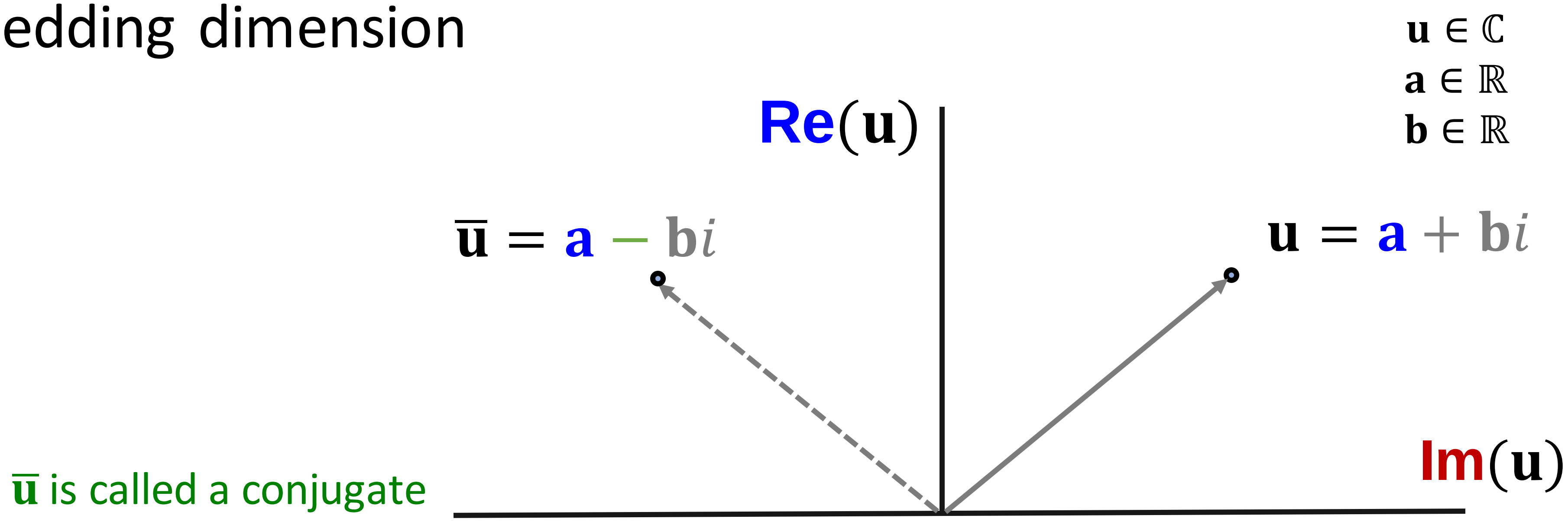
- **Composition Relations:**

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

  - **Example**: My mother's husband is my father.
- **DistMult** can model composition relations ✓
  - DistMult uses matrix multiplication / inner product
  - Composition can correspond to chain matrix multiplication

ComplEx

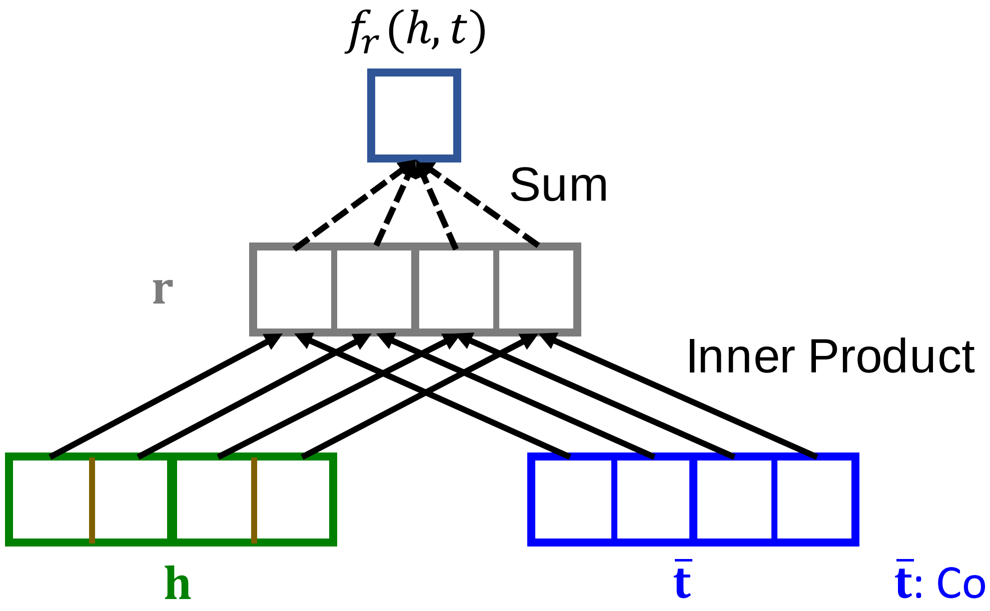
- Based on Distmult, **ComplEx** embeds entities and relations in **Complex vector space**
- **ComplEx**: model entities and relations using vectors in $\mathbb{C}^k$
- k is the embedding dimension



Trouillon et al, Complex Embeddings for Simple Link Prediction, ICML 2016

ComplEx

- **ComplEx**: model entities and relations using vectors in $\mathbb{C}^k$
- For each triple (h, r, t), $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{C}^k$ are the embedding vectors
- **Score function** $f_r(h,t) = \mathrm{Re}(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i)$



$\bar{\mathbf{t}}$: Conjugate of $\mathbf{t}$

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 $\mathbf{Im}(\mathbf{r}) = \mathbf{0}$**, we have
    - $f_r(h,t) = \mathrm{Re}(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i) = \sum_i \mathrm{Re}(\mathbf{r}_i \cdot \mathbf{h}_i \cdot \bar{\mathbf{t}}_i)$
      $= \sum_i \mathbf{r}_i \cdot \mathrm{Re}(\mathbf{h}_i \cdot \bar{\mathbf{t}}_i) = \sum_i \mathbf{r}_i \cdot \mathrm{Re}(\bar{\mathbf{h}}_i \cdot \mathbf{t}_i)$
      $= \sum_\mathrm{i} \mathrm{Re}(\mathbf{r}_\mathrm{i} \cdot \bar{\mathbf{h}}_\mathrm{i} \cdot \mathbf{t}_\mathrm{i}) = f_r(t,h)$

Antisymmetric Relations in ComplEx

- **Antisymmetric Relations:**

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

  - **Example**: Hypernym
- **ComplEx** can model antisymmetric relations ✓
  - The model is expressive enough to learn
    - $f_r(h,t) = \mathrm{Re}(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i)$
    - $f_r(t,h) = \mathrm{Re}(\sum_i \boldsymbol{t}_i \cdot \mathbf{r}_i \cdot \bar{\boldsymbol{h}}_i)$
  - $r(h,t)$ and $r(t,h)$ can have different scores in ComplEx, due to the asymmetric modeling using complex conjugate.

Inverse Relations in ComplEx

- **Inverse** Relations:

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

  - **Example** : (Father, Son)
- **ComplEx** can model inverse relations ✓
  - $\mathbf{r}_1 = \bar{\mathbf{r}}_2$
  - Complex conjugate of $\mathbf{r}_2 = \underset{\mathbf{r}}{\operatorname{argmax}} \operatorname{Re}(<\mathbf{h}, \mathbf{r}, \bar{\mathbf{t}}>)$:

    $\bar{\mathbf{r}}_2$ is exactly $\mathbf{r}_1 = \underset{\mathbf{r}}{\operatorname{argmax}} \operatorname{Re}(<\mathbf{t}, \mathbf{r}, \bar{\mathbf{h}}>)$.
  - Note: $\operatorname{Re}(<\mathbf{h}, \mathbf{r}, \bar{\mathbf{t}}>) = \operatorname{Re}(<\mathbf{t}, \bar{\boldsymbol{r}}, \bar{\mathbf{h}}>)$

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** shares the same property with **DistMult**

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RotatE

- **RotatE:** represent triple (h, r, t) in complex vector space, i.e.,$\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{C}^k$
- k is the embedding dimension
- Define each relation $\mathbf{r}$ as an element-wise rotation from the head $\mathbf{h}$ to the tail $\mathbf{t}$

$$\mathbf{t} = \mathbf{h} \circ \mathbf{r}, \text{ where } |r_j| = 1$$

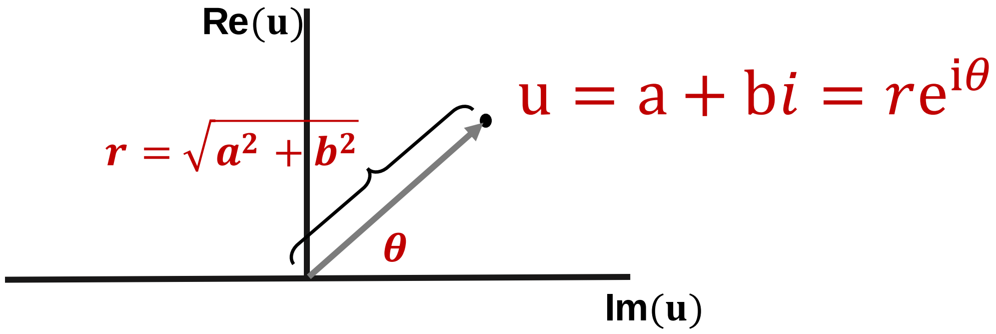
  - $\circ$ is the **Hadmard** (element-wise) product (i.e., $t_j = h_j \cdot r_j$ for each j).
  - j denotes the j-th dimension, t_j, h_j , $r_j \in \mathbb{C}$.

Sun et al, RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space, ICLR 2019

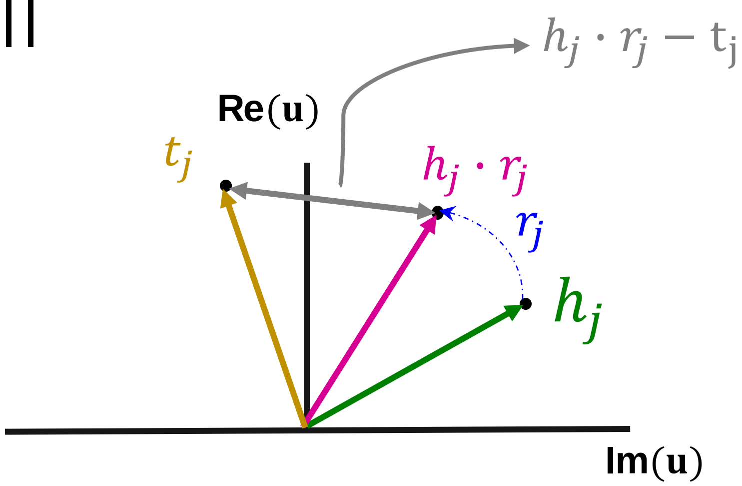
Relation as Rotation

- Since $|r_j| = 1$, r_j can also be represented as $r_j = e^{i\theta_{r,j}}$, $\theta_{r,j}$ is the **phase angle**
- $r_j = e^{i\theta_{r,j}}$ and $t_j = h_j \cdot r_j$ means h_j is rotated $\theta_{r,j}$ clockwise in the complex space
- Define **the score function** of RotatE as

$$f_r(\mathbf{h}, \mathbf{t}) = -||\mathbf{h} \circ \mathbf{r} - \mathbf{t}||$$



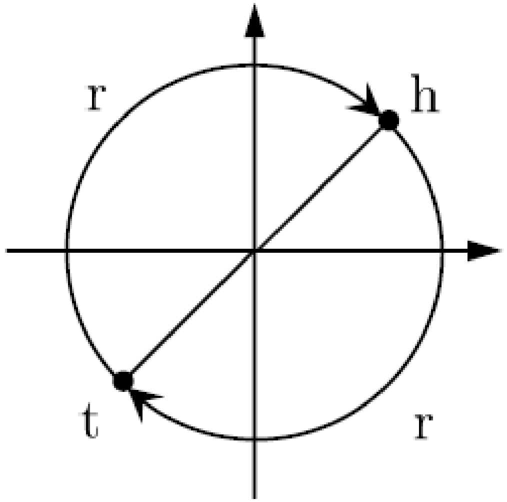
r: magnitude
θ: phase angle



Symmetric and Antisymmetric in RotatE

- **RotatE can model symmetric and antisymmetric Relations**
- **Symmetric Relations:**

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



- r is **symmetric** if and only if $r_j = \pm 1$, i.e., $\theta_{r,j} = 0 \; or \; \pi$
- An example on the space of $\mathbb{C}$
  - $r_j = -1$ or $\theta_{r,j} = \pi$

- **Antisymmetric Relations:** $r(h,t) \Rightarrow \neg r(t,h) \quad \forall h,t$
- r is **antisymmetric** if and only if $\mathbf{r} \circ \mathbf{r} \neq \mathbf{1}$, i.e., $\theta_{r,j} \neq 0$ and π

Other Relations in RotatE

- **RotatE can model Inverse and Composition relations**
- **Inverse Relations:** $r_2(h,t) \Rightarrow r_1(t,h)$
- Two relations r_1 and r_2 are **inverse** if and only if $\mathbf{r}_2 = \bar{\mathbf{r}}_1$, i.e., $\theta_{2,j} = -\theta_{1,j}$

- **Composition Relations:** $r_1(x,y) \wedge r_2(y,z) \Rightarrow r_3(x,z) \quad \forall x,y,z$
- relation $\mathbf{r_3} = \mathbf{e^{i\theta_3}}$ is a **composition** of two relations $\mathbf{r_1} = \mathbf{e^{i\theta_1}}$ and $\mathbf{r_2} = \mathbf{e^{i\theta_2}}$ if only if $\mathbf{r_3} = \mathbf{r_1} \circ \mathbf{r_2}$,
  - i.e., $\theta_{3,j} = \theta_{1,j} + \theta_{2,j}$.
  - $\theta_{k,j}$ is the k-th dimension of $\boldsymbol{\theta_k}$

Limitations of RotatE

- **1-to-N Relations:**
  - **Example**: If (h, r, t_1) and (h, r, t_2) exist in the knowledge graph
- RotatE cannot model 1-to-N relations
- if $\mathbf{t_1} = \mathbf{h} \circ \mathbf{r}$ and $\mathbf{t_2} = \mathbf{h} \circ \mathbf{r}$,

$$\Rightarrow t_{1,j} = \mathrm{h_j} \cdot r_j;\ t_{2,j} = \mathrm{h_j} \cdot r_j \text{ for each } j$$

$$\Rightarrow \mathbf{t_1} = \mathbf{t_2}\,!$$

Content

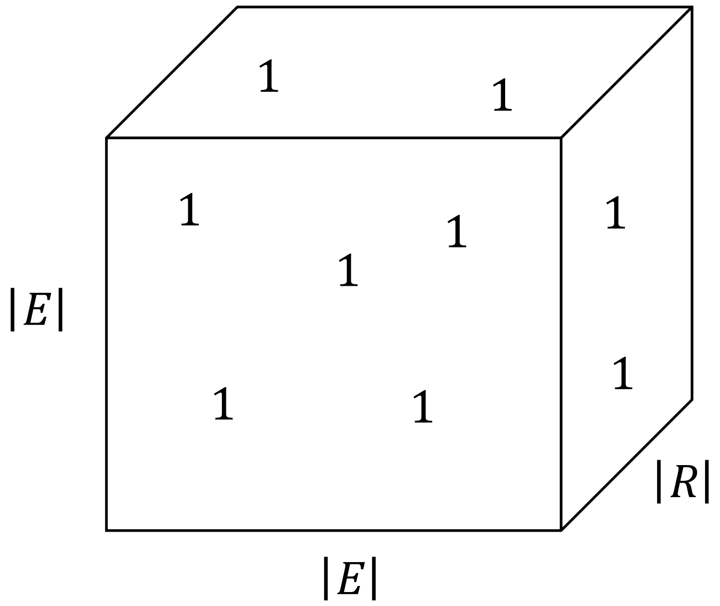
- Introduction: Knowledge Graph

- **Knowledge Graph Embedding Models**
  - TransE
  - DistMult & ComplEx
  - RotatE
  - **TuckER**

TuckER

- An alternative view of a knowledge graph: **sparse binary adjacency tensor** representation of known fact.
- E is the entity set, R is the relation set
- If (h, r, t) exists in KG, then

$$tensor(h, r, t) = 1$$



Balazević et al, TuckER: Tensor Factorization for Knowledge Graph Completion , EMNLP 2019

Backgournd: Tucker Decomposition

- **Tucker decomposition** decomposes a tensor into a set of matrices and **a smaller core tensor.**
- In three-mode case, given the original tensor $\mathcal{X} \in \mathbb{R}^{I \times J \times K}$, Tucker decomposition outputs a tensor $\mathcal{Z} \in \mathbb{R}^{P \times Q \times R}$ and three matrices $\boldsymbol{A} \in \mathbb{R}^{I \times P}$, $\boldsymbol{B} \in \mathbb{R}^{J \times Q}$, $\boldsymbol{C} \in \mathbb{R}^{K \times R}$:

$$\mathcal{X} \approx \mathcal{Z} \times_1 \boldsymbol{A} \times_2 \boldsymbol{B} \times_3 \boldsymbol{C}$$

  - $\times_n$ indicates the tensor product along the n-th mode
  - Elements of the ***core tensor*** $\mathcal{Z}$, $\mathcal{Z}(p, q, r)$ show the interaction level between the component $\boldsymbol{A}[p], \boldsymbol{B}[q]$ and $\boldsymbol{C}[r]$. $[i]$ denotes the i-th column
  - the ***core tensor*** $\mathcal{Z}$ can be considered as a compressed version of $\mathcal{X}$

Tucker decomposition for KG

- **TuckER** uses **Tucker decomposition** for Knowledge Graph Completion
- entity embedding matrix $\boldsymbol{E} \in \mathbb{R}^{n_e \times d_e}$ and relation embedding matrix $\boldsymbol{R} \in \mathbb{R}^{n_r \times d_r}$
  - n_e, n_r represent the number of entities and relations
  - d_e, d_r represent the dimensionality of entity embedding and relation embedding
- Three matrices in Tucker: $\boldsymbol{A} = \boldsymbol{C} = \boldsymbol{E} \in \mathbb{R}^{n_e \times d_e}$ and $\boldsymbol{B} = \boldsymbol{R} \in \mathbb{R}^{n_r \times d_r}$
- **Scoring function for TuckER:**

$$\phi(\mathbf{h}, \mathbf{r}, \mathbf{t}) = \boldsymbol{\mathcal{W}} \times_1 \mathbf{h} \times_2 \mathbf{r} \times_3 \mathbf{t}$$

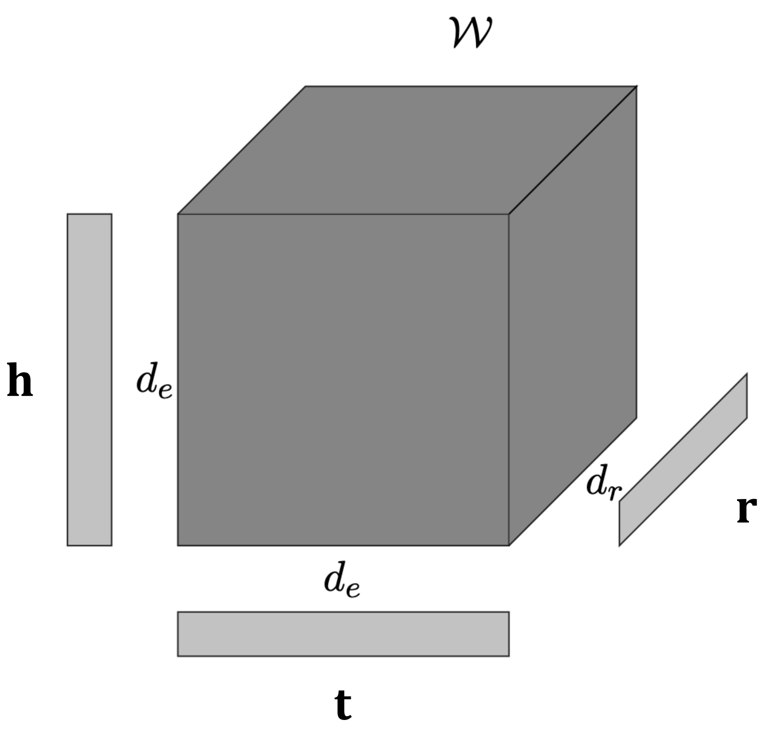
  - $\mathbf{h}, \mathbf{t} \in \mathbb{R}^{d_e}$ are the rows of $\boldsymbol{E}$, $\mathbf{r} \in \mathbb{R}^{d_r}$ is the row of $\boldsymbol{R}$
  - $\boldsymbol{\mathcal{W}} \in \mathbb{R}^{d_e \times d_r \times d_e}$ is the core tensor
  - d_e, d_r can be different in TuckER

TuckER architecture

- **Scoring function:**

$$\phi(\mathbf{h}, \mathbf{r}, \mathbf{t}) = \boldsymbol{\mathcal{W}} \times_1 \mathbf{h} \times_2 \mathbf{r} \times_3 \mathbf{t}$$

- Apply logistic sigmoid to socre $\phi(\mathbf{h}, \mathbf{r}, \mathbf{t})$ to obtain the predicted probability of triple being true
- The core tensor $\boldsymbol{\mathcal{W}}$ can be viewed as a shared pool of "prototype" relation matrices, which are linearly combined using the parameters in each relation embedding $\mathbf{r}$.



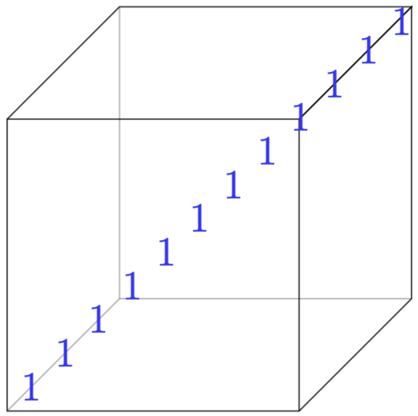
Relation to Previous Models

- Recap: Score function of **DistMulti**:

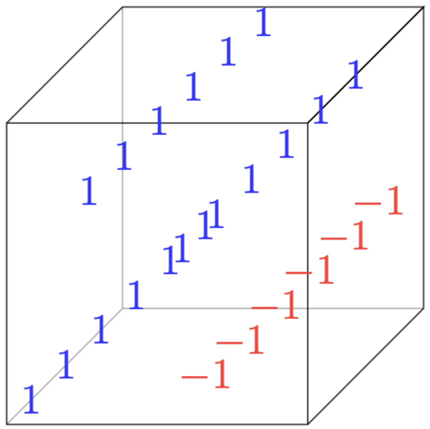
$$f_r(h,t) = <\mathbf{h},\mathbf{r},\mathbf{t}> = \sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \mathbf{t}_i \,; \quad \mathbf{h},\mathbf{r},\mathbf{t} \in \mathbb{R}^k$$

- Score function of **ComplEx**:

$$f_r(h,t) = \mathrm{Re}\left(\sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \bar{\mathbf{t}}_i\right); \quad \mathbf{h},\mathbf{r},\mathbf{t} \in \mathbb{C}^k$$



Core tensor $\mathcal{W} \in \mathbb{R}^{d_e \times d_r \times d_e}$ for DistMult



Core tensor $\mathcal{W} \in \mathbb{R}^{2d_e \times 2d_r \times 2d_e}$ for ComplEx

Expressiveness of All Models

- Properties and expressive power of different KG completion methods:

Model	Score	Embedding	Sym.	Antisym.	Inv.	Compos.	1-to-N
TransE	$-\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{R}^k$	✗	✓	✓	✓	✗
DistMult	$<\mathbf{h},\mathbf{r},\mathbf{t}>$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{R}^k$	✓	✗	✗	✓	✓
ComplEx	$\mathrm{Re}(<\mathbf{h},\mathbf{r},\bar{\mathbf{t}}>)$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{C}^k$	✓	✓	✓	✓	✓
RotatE	$-\|\mathbf{h}\circ\mathbf{r}-\mathbf{t}\|$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{C}^k$	✓	✓	✓	✓	✗
TuckER	$\mathcal{W}\times_1\mathbf{h}\times_2\mathbf{r}\times_3\mathbf{t}$	$\mathbf{h},\mathbf{t}\in\mathbb{R}^{d_e}$, $\mathbf{r}\in\mathbb{R}^{d_r}$	✓	✓	✓	✓	✓

- ComplEx extends DistMult by introducing complex embeddings
- RotatE can degenerate into TransE (See proof in original paper, Appendix F)
- TuckER uses tensor factorization to propose a fully expressive knowledge graph model

Today's Summary

- Different KGs may have **drastically different relation patterns**!
- **Modeling relation patterns** is critical for knowledge base completion
  - Symmetric/Antisymmetric, Inverse, composition, 1-to-N
- There is not a general embedding that works for all KGs, use the **table** to select models
- In practice: try **TransE** for a quick run if the target KG does not have much symmetric relations, then use more expressive models, e.g., **DistMult, ComplEx**, **RotatE, TuckER**