Knowledge Graphs

ACMS 80770: Deep Learning with Graphs

Instructor: Navid Shervani-Tabar

Department of Applied and Comp Math and Stats

UNIVERSITY OF NOTRE DAME

Knowledge Graph

- Real world **information** can be stored in the form of **entities** and the **relationships** between them.
- To that end, a fact can be represented using triple

$$(subject, predicate, object)$$

  where $subject$ and $object$ are entities and $predicate$ is their relation.
- The **set** of these triples represents **knowledge**.

Knowledge Graph

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Chandler Bing	characterIn	Friends
Friends	genre	Sitcom

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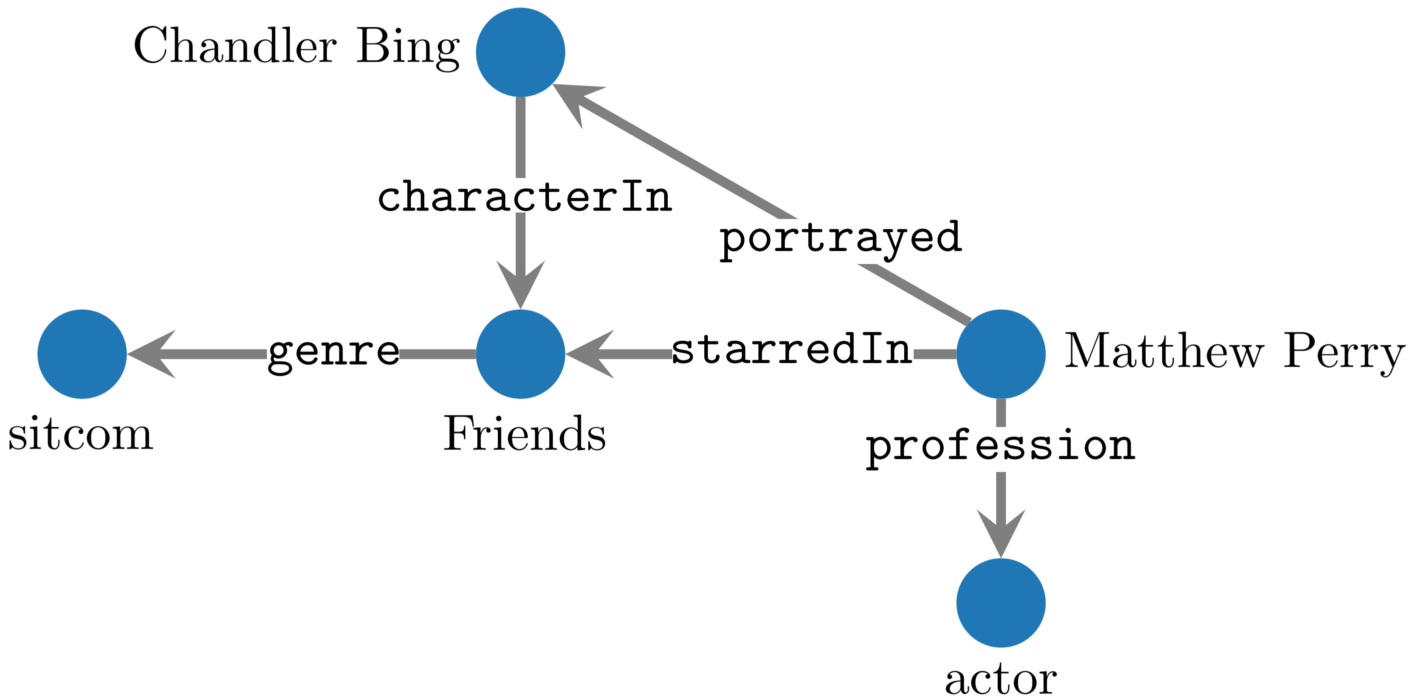
- Each 3-tuple (v_h, τ, v_t) specifies a **fact** that holds between nodes v_h and v_t.
- This graph-structured representation of information is known as **knowledge graph**.
- Knowledge graphs can be used to represent the **factual information** and the **knowledge of the real world**.

Knowledge Graph

➢ We can represent the set of triplets in our example in a **graph-structured** manner.



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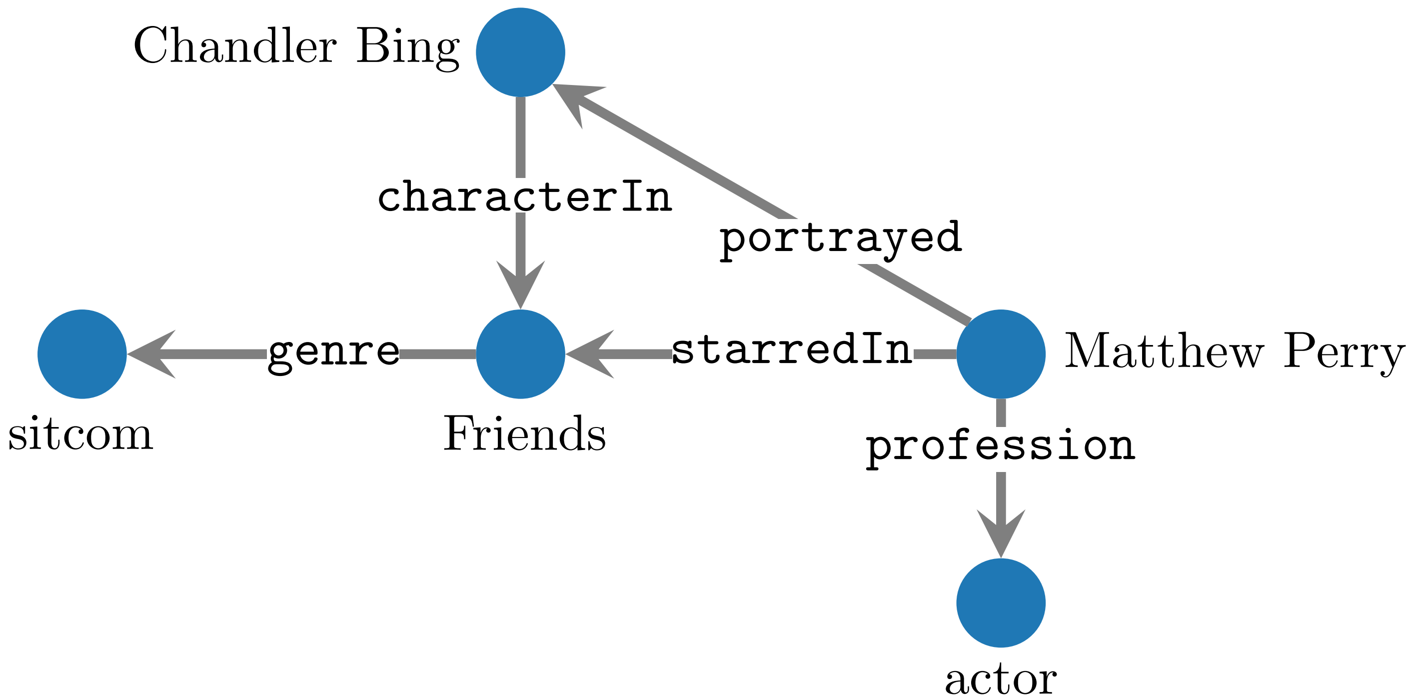

- **Knowledge graphs** are consist of various types of nodes and edges and therefore are **heterogenous** graphs.

Heterogeneous Graphs

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- Each edge is defined by $(u, \tau, v) \in \mathrm{E}$, where τ is the type of the edge.

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- Each edge is defined by $(u, \tau, v) \in \mathrm{E}$, where τ is the type of the edge.
- In a heterogeneous graph

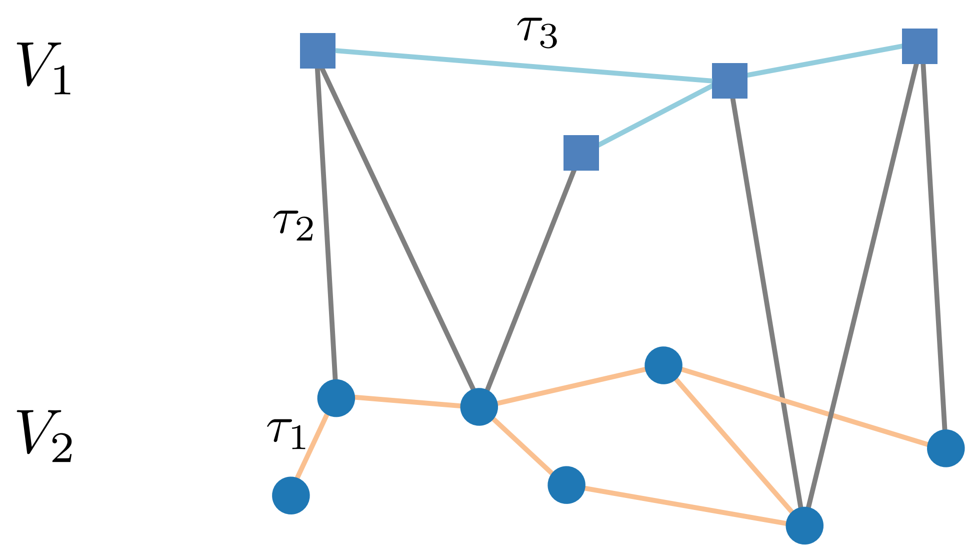
$$V = V_1 \cup \ldots \cup V_k, V_i \cap V_j = \emptyset, \forall i \neq j$$

  Here, V_j is set of **nodes** with **type** j.
- Edges of specific type τ_i usually only connect nodes of certain types.

$$(u, \tau_i, v) \in \varepsilon \rightarrow u \in V_j, v \in V_k$$

Heterogeneous Graphs

- Polypharmacy side-effect graph



τ_1 : Protein-protein interaction

τ_2 : Protein-drug interaction

τ_3 : Polypharmacy side-effect

V_1 : Drugs

V_2 : Proteins

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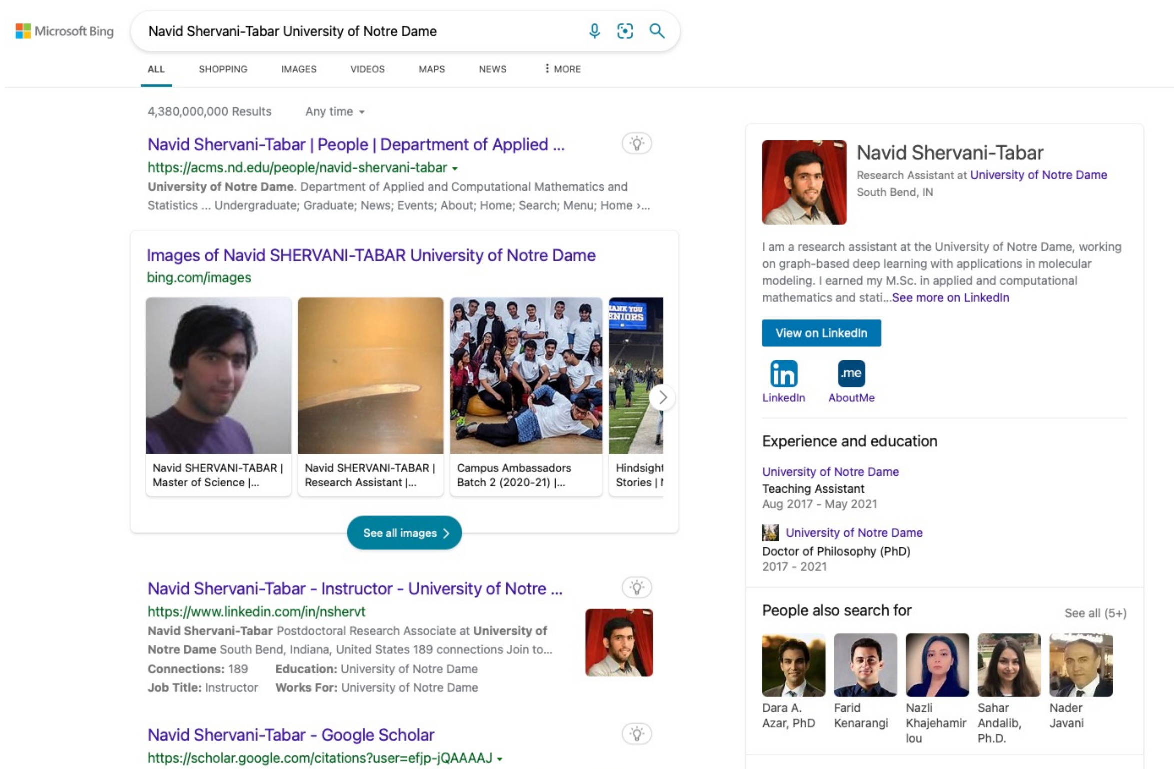
- AstraZeneca: Genomic research

Knowledge Graph

➤ Web Search

- Google knowledge graph
- Bing knowledge graph (Satori)



KG Completion

- Human knowledge about the relation between different entities is notoriously **incomplete**.
- The “place of birth” is **missing** for 71% of the people on the Freebase knowledge graph.
- As a result, knowledge graphs are often riddled with **missing edges**.

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- As a result, knowledge graphs are often riddled with **missing edges**.
- **Knowledge graph completion** approaches are the set of techniques aiming to fill the missing edges.
- In addition, they can be used to **predict new facts** about the world.

KG Completion

- In general, the knowledge graph completion involves **link prediction** problem, while in some cases we may deal with **node classification** as well.
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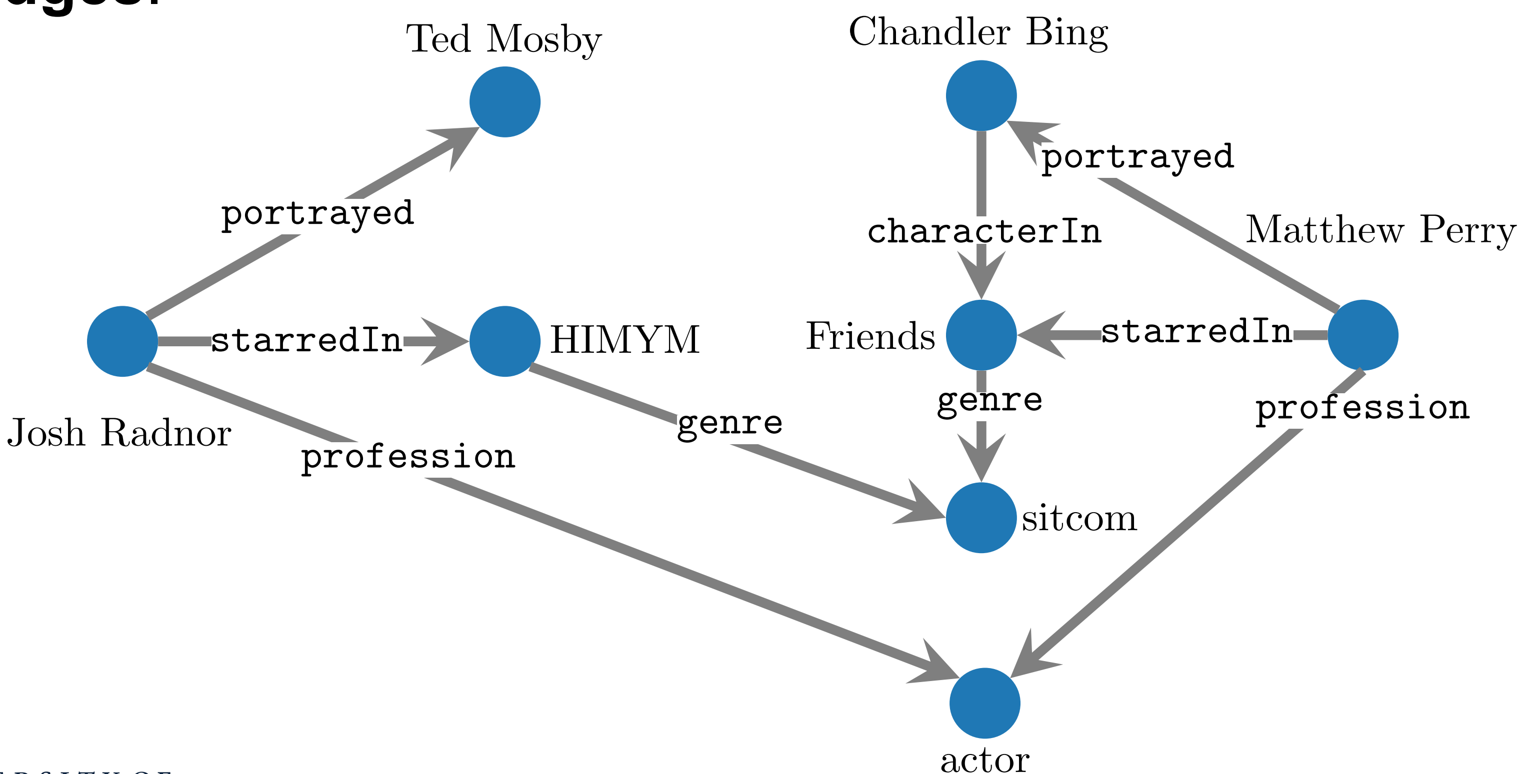

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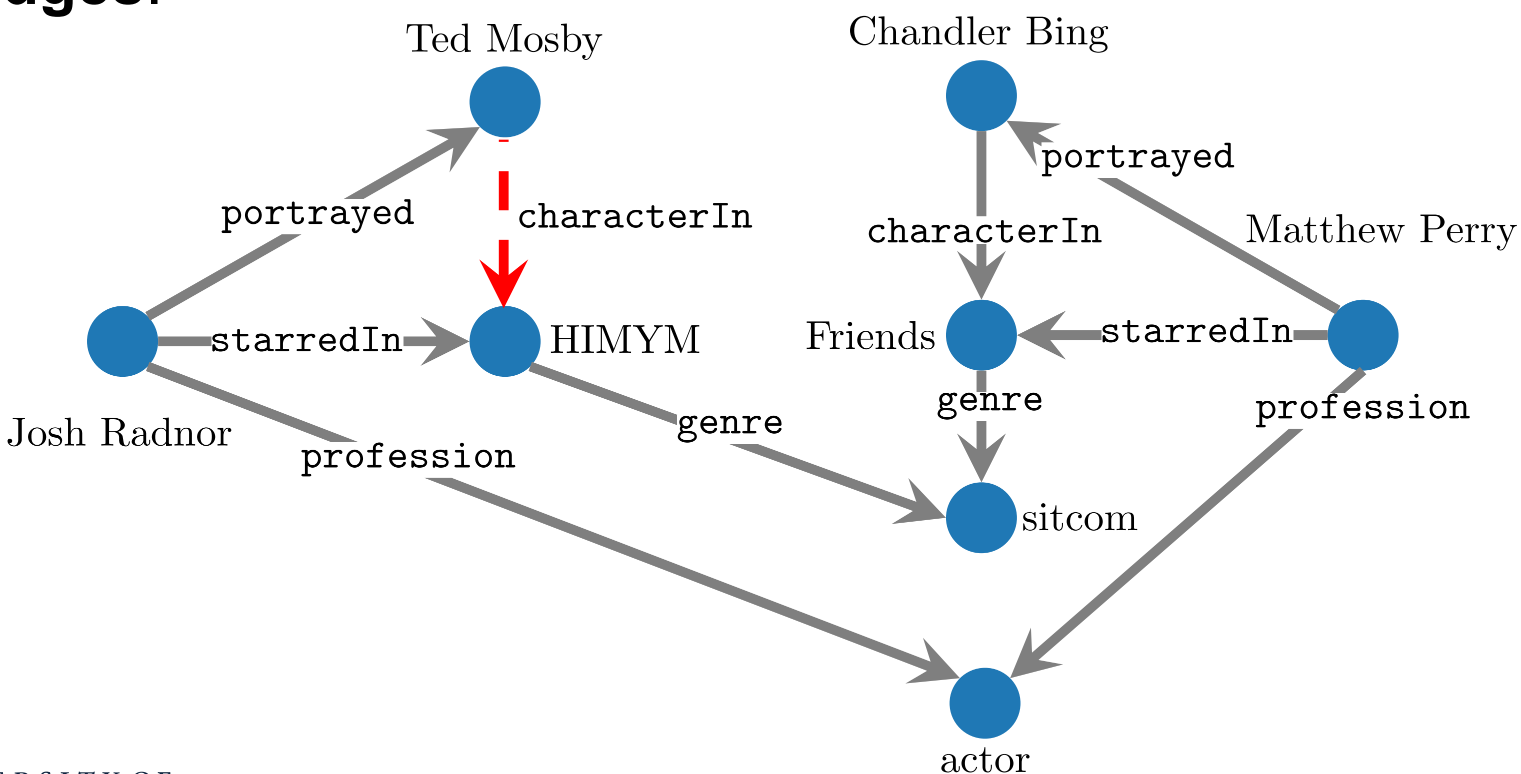
  - 

KG Embeddings

- In general, the knowledge graph completion involves **link prediction** problem, while in some cases we may deal with **node classification** as well.

- Link prediction refers to predicting existence of **missing edges**.

- To tackle this link prediction problem with machine learning models, we use **knowledge graph embedding** techniques to construct graph embeddings.

- These embeddings consist of **entity embeddings** $\boldsymbol{z}_h$ and $\boldsymbol{z}_t$ for nodes $v_i, v_j \in V$, and **relational embedding** r_τ that relates a pair of entities

Relational Patterns

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- (Jesus, *childOf*, Mary)⇔(Mary, *parentOf*, Jesus)

Relational Patterns

- **Compositionality**: Relation τ_3 is composed of relations τ_1 and τ_2 if for all $v_i, v_j, v_k \in \mathrm{V}$,

$$(v_i, \tau_1, v_j) \in E \ \wedge \ (v_j, \tau_2, v_k) \Longrightarrow (v_i, \tau_3, v_k) \in E$$

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  - College varsity teams draft players from students enrolled in that college.

(Ian Book, *draftedBy*, Fighting Irish)∧ (Fighting Irish, *school*, Notre Dame)

→ (Ian Book, *enrolledAt*, Notre Dame)

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- In the shallow embedding approach, we need to define a **loss**, a **similarity** measure, and a **decoder**.

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- In the shallow embedding approach, we need to define a **loss**, a **similarity** measure, and a **decoder**.
- Learning **node embeddings** involves reconstructing the local structure of a node v_i given its embedding $\boldsymbol{z}_i$.
- While learning node embeddings, we used various node-node **similarity measures** to define this **local structure**.

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- In the shallow embedding approach, we need to define a **loss**, a **similarity** measure, and a **decoder**.
- Learning **node embeddings** involves reconstructing the local structure of a node v_i given its embedding $\boldsymbol{z}_i$.
- While learning node embeddings, we used various node-node **similarity measures** to define this **local structure**.
- Similarly, in knowledge graph completion, we aim to **reconstruct the relation between nodes** v_i and v_j given the embeddings $\boldsymbol{z}_i$ and $\boldsymbol{z}_j$.

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- Therefore, we define the **decoder** as a map

$$f_d: R^d \times \mathcal{R} \times R^d \rightarrow R^+$$

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  to predict existence of edge types between nodes v_i and v_j.
- Given node embeddings $\boldsymbol{z}_i$ and $\boldsymbol{z}_j$ and relational embedding $\boldsymbol{r}_\tau$, a decoder f_d evaluates the plausibility of the edge type τ between nodes v_i and v_j.

Multi-relational Decoder

- When **training** the model for the link prediction task, we predict the **plausibility** of the relational data. These relations have been extracted from the external sources.
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- This **closeness** quantifies the probability of the two entities being in a **relationship**.

$$f_d\left(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t\right) = -d\left(\boldsymbol{z}_h + \boldsymbol{r}_\tau, \boldsymbol{z}_t\right)$$

TransE

- The most basic translational model is called **TransE**.
- Given a tuple (v_h, τ, v_t) representing a fact, TransE learns entity and relational embeddings $\boldsymbol{z}_h$, $\boldsymbol{z}_t$, and $\boldsymbol{r}_\tau$ so as to minimize the distance between $\boldsymbol{z}_h + \boldsymbol{r}_\tau$ and $\boldsymbol{z}_t$.
- TransE **scores** (v_h, τ, v_t) based on closeness of $\boldsymbol{z}_h + \boldsymbol{r}_\tau$ and $\boldsymbol{z}_t$.

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- TransE **scores** (v_h, τ, v_t) based on closeness of $\boldsymbol{z}_h + \boldsymbol{r}_\tau$ and $\boldsymbol{z}_t$.
- Mathematically put, TransE defines the decoder as

$$f_d\left(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t\right) = -\left\|\boldsymbol{z}_h + \boldsymbol{r}_\tau - \boldsymbol{z}_t\right\|$$

  where $\boldsymbol{r}_\tau \in \mathbb{R}^d$ is the relational embedding and $\boldsymbol{z}_h, \boldsymbol{z}_t \in \mathbb{R}^d$ are entity embeddings.
- Therefore, the distance between the translated entity embedding $\boldsymbol{z}_h + \boldsymbol{r}_\tau$ and the entity embedding $\boldsymbol{z}_t$ represents the **likelihood** of **existence** of relation type τ between v_h and v_t.

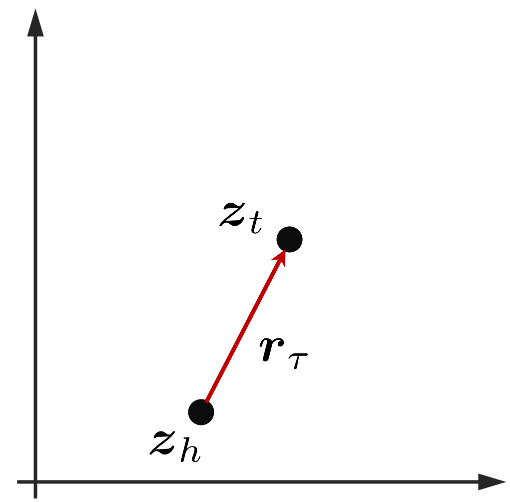
TransE: Relational Patterns

- **Symmetry:**

$$\boldsymbol{z}_h + \boldsymbol{r}_\tau = \boldsymbol{z}_t$$
$$\boldsymbol{z}_t + \boldsymbol{r}_\tau = \boldsymbol{z}_h$$

$$\implies \quad \boldsymbol{r}_\tau = 0, \quad \boldsymbol{z}_h = \boldsymbol{z}_t$$

Cannot.



- **Anti-Symmetry**:

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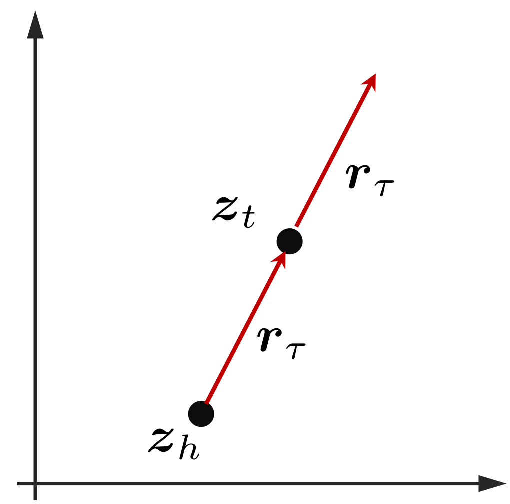
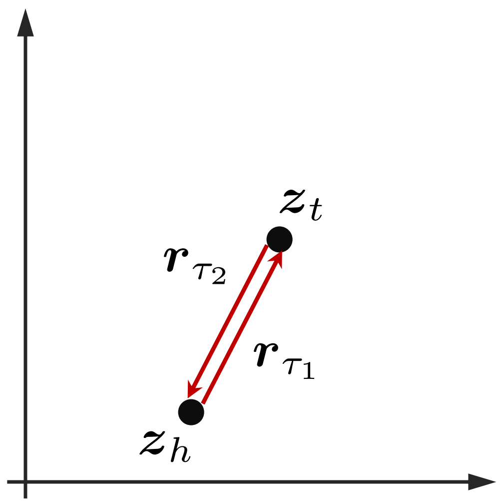


TransE: Relational Patterns

- Inverse:

$$\boldsymbol{z}_h + \boldsymbol{r}_{\tau_1} = \boldsymbol{z}_t$$
$$\boldsymbol{z}_t + \boldsymbol{r}_{\tau_2} = \boldsymbol{z}_h$$

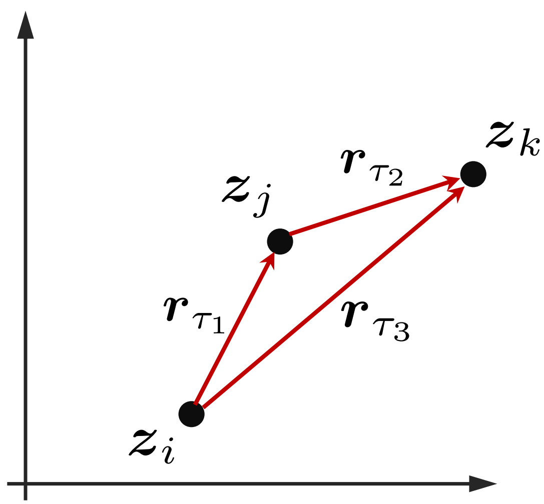
$$\implies \quad \boldsymbol{r}_{\tau_1} = -\boldsymbol{r}_{\tau_2}$$



- Compositionality:

$$\boldsymbol{z}_i + \boldsymbol{r}_{\tau_1} = \boldsymbol{z}_j$$
$$\boldsymbol{z}_j + \boldsymbol{r}_{\tau_2} = \boldsymbol{z}_k$$
$$\boldsymbol{z}_i + \boldsymbol{r}_{\tau_3} = \boldsymbol{z}_k$$

$$\implies \quad \boldsymbol{r}_{\tau_1} + \boldsymbol{r}_{\tau_2} = \boldsymbol{r}_{\tau_3}$$



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- To address these issues, many **variants** of the TransE model have been proposed.
- **TransR** is defined based on the intuition that, entities have **various aspects**, and different relational spaces should represent different aspect of these entities.
- TransR approach represents each relation type τ in a **distinct vector space**.

$$\boldsymbol{z}_h^{\tau} = \mathbf{M}_{\tau}\boldsymbol{z}_h, \qquad \boldsymbol{z}_t^{\tau} = \mathbf{M}_{\tau}\boldsymbol{z}_t$$

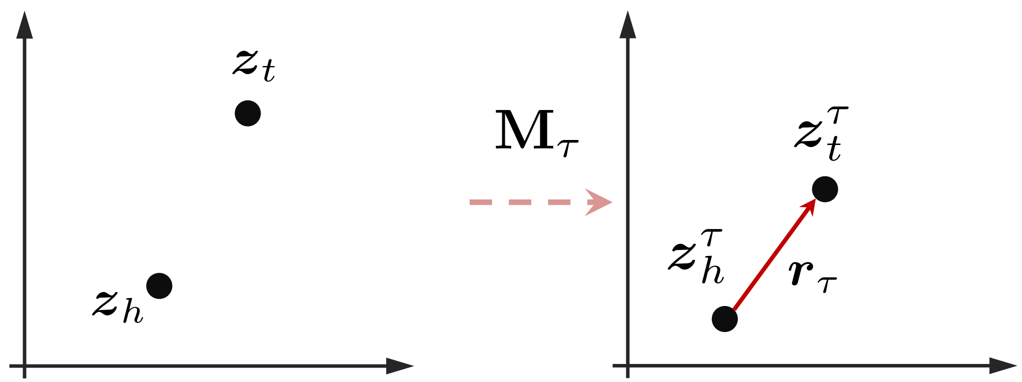
- TransR uses relation-specific **projection** matrices M_τ to project node embeddings onto the relation-specific vector space before **translating** them.

TransR

- We can formulate the TransR model as

$$f_d\left(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t\right) = -\left\|\mathbf{M}_\tau \boldsymbol{z}_h + \boldsymbol{r}_\tau - \mathbf{M}_\tau \boldsymbol{z}_t\right\|$$

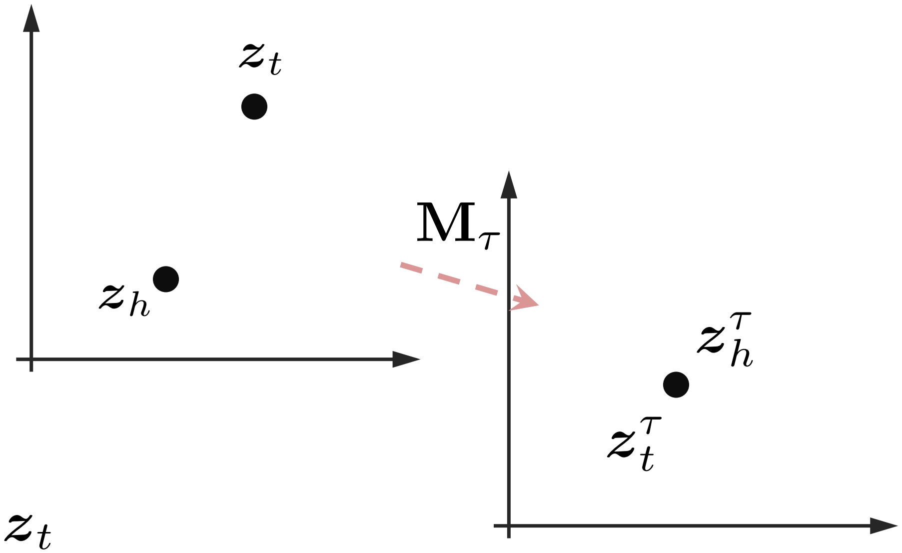
where $\boldsymbol{z}_h, \boldsymbol{z}_t \in \mathbb{R}^d$, $\boldsymbol{r}_\tau \in \mathbb{R}^k$ and $\mathbf{M}_\tau \in \mathbb{R}^{k\times d}$.



TransR: Relational Patterns

- **Symmetry:**

$$\mathbf{M}_\tau \boldsymbol{z}_h + \boldsymbol{r}_\tau = \mathbf{M}_\tau \boldsymbol{z}_t$$
$$\mathbf{M}_\tau \boldsymbol{z}_t + \boldsymbol{r}_\tau = \mathbf{M}_\tau \boldsymbol{z}_h$$
$$\Longrightarrow \quad \boldsymbol{r}_\tau = 0$$
$$\mathbf{M}_\tau \boldsymbol{z}_h = \mathbf{M}_\tau \boldsymbol{z}_t$$



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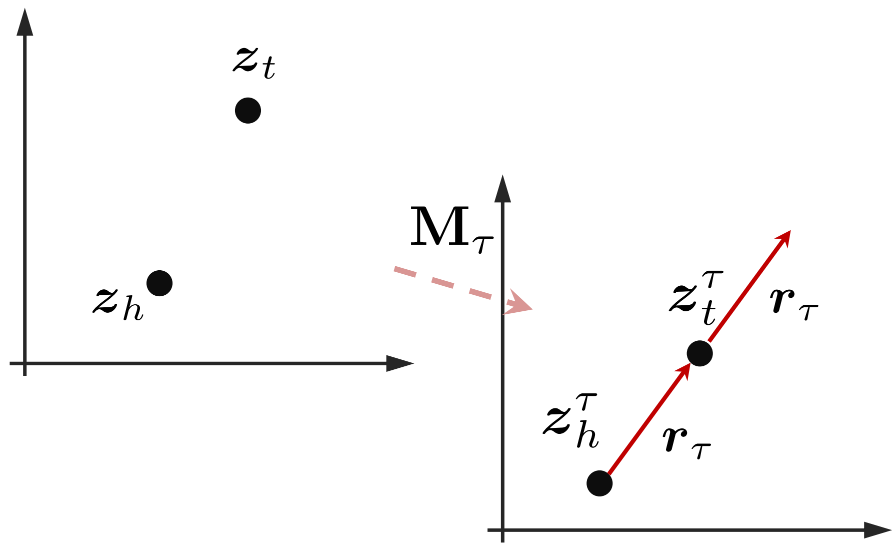


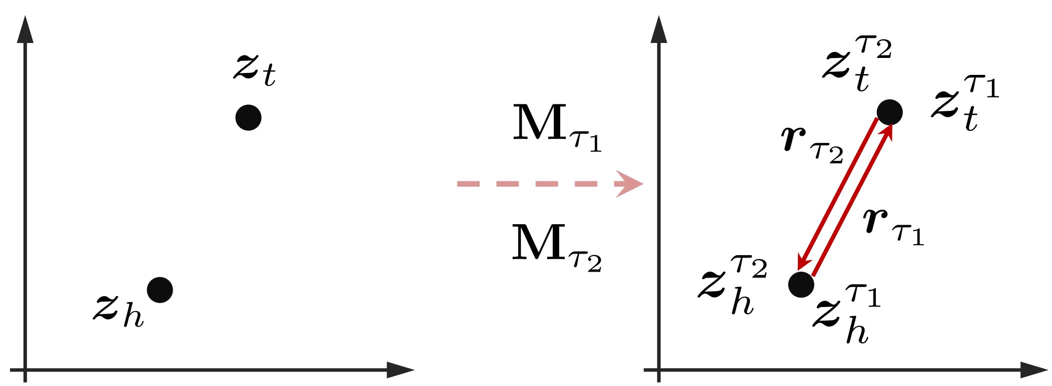
TransR: Relational Patterns

- Inverse:

$$\mathbf{M}_{\tau_1}\boldsymbol{z}_h + \boldsymbol{r}_{\tau_1} = \mathbf{M}_{\tau_1}\boldsymbol{z}_t$$
$$\mathbf{M}_{\tau_2}\boldsymbol{z}_t + \boldsymbol{r}_{\tau_2} = \mathbf{M}_{\tau_2}\boldsymbol{z}_h$$

- If $M_{\tau_1} = M_{\tau_2}$, we can project entity embeddings to the same relation specific space, and we can use

$$\boldsymbol{r}_{\tau_1} = -\boldsymbol{r}_{\tau_2}$$



TransR: Relational Patterns

➢ **Compositionality:**

$$\mathbf{M}_{\tau_1}\boldsymbol{z}_i + \boldsymbol{r}_{\tau_1} = \mathbf{M}_{\tau_1}\boldsymbol{z}_j$$
$$\mathbf{M}_{\tau_2}\boldsymbol{z}_j + \boldsymbol{r}_{\tau_2} = \mathbf{M}_{\tau_2}\boldsymbol{z}_k$$
$$\mathbf{M}_{\tau_3}\boldsymbol{z}_i + \boldsymbol{r}_{\tau_3} = \mathbf{M}_{\tau_3}\boldsymbol{z}_k$$

❖ Since translations between relation specific spaces are not defined, we can't represent compositional patterns using TransR.

RotatE

- RotatE, learns translational embeddings in the **complex space**.
- In this method, relations are modeled as **element-wise rotations** in the complex vector space.
- Based on Euler's identity

$$e^{i\theta} = \cos\theta + i\sin\theta$$

A unitary complex number can represent a relation in the complex plane.

- Motivated by Euler's identity, RotatE defines the decoder as

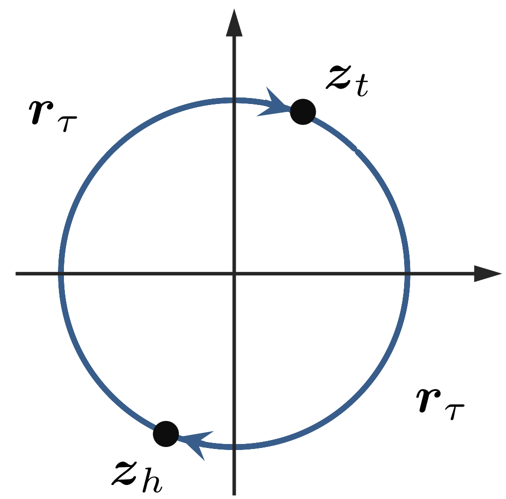
$$f_d\left(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t\right) = -\left\|\boldsymbol{z}_h \odot \boldsymbol{r}_\tau - \boldsymbol{z}_t\right\|$$

where $\boldsymbol{z}_h, \boldsymbol{z}_t, \boldsymbol{r}_\tau \in \mathbb{C}^d$ and $|[\boldsymbol{r}_\tau]_i| = 1$.

RotatE: Relational Patterns

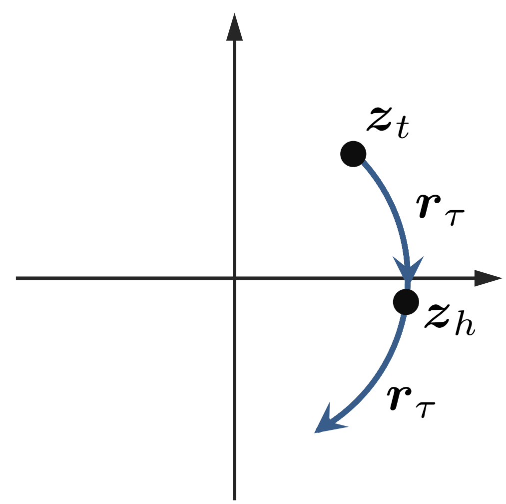
- Symmetry:

$$\boldsymbol{z}_h \odot \boldsymbol{r}_\tau = \boldsymbol{z}_t$$
$$\boldsymbol{z}_t \odot \boldsymbol{r}_\tau = \boldsymbol{z}_h$$
$$\Longrightarrow \quad [\boldsymbol{r}_\tau]_j = -1$$



- Anti-Symmetry:

$$\boldsymbol{z}_h \odot \boldsymbol{r}_\tau = \boldsymbol{z}_t$$
$$\boldsymbol{z}_t \odot \boldsymbol{r}_\tau \neq \boldsymbol{z}_h$$



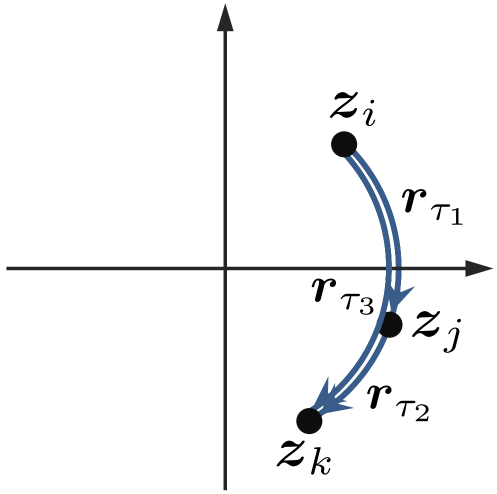
RotatE: Relational Patterns

- Inverse:

$$\boldsymbol{r}_{\tau_2} = \bar{\boldsymbol{r}}_{\tau_1}$$

- Compositionality:

$$\theta_3 = \theta_2 + \theta_1$$



Tensor Decomposition Models

- Another group of decoding models are tensor decomposition models.
- Here we review the following methods
  - RESCAL
  - DistMult
  - ComplEx

RESCAL

- RESCAL is one of the earliest learning approaches for multi-relational embeddings.
- RESCAL defines a decoder based on **pair-wise interaction** of the embeddings

$$f_d\left(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t\right) = \boldsymbol{z}_h^T \boldsymbol{r}_\tau \boldsymbol{z}_t$$

  where $\boldsymbol{r}_\tau \in \mathbb{R}^{d \times d}$ is a learnable **relation-specific matrix** and $\boldsymbol{z}_h, \boldsymbol{z}_t \in \mathbb{R}^d$ are entity embeddings.

- Element $[\boldsymbol{r}_\tau]_{i,j}$ indicates how much embedding dimensions $[\boldsymbol{z}_h]_i$ and $[\boldsymbol{z}_t]_j$ interact in the relation type τ.

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- Element $[\boldsymbol{r}_\tau]_{i,j}$ indicates how much embedding dimensions $[\boldsymbol{z}_h]_i$ and $[\boldsymbol{z}_t]_j$ interact in the relation type τ.
- While RESCAL can infer the discussed relational patterns, it is **computationally expensive**.

DistMult

- DistMult method defines the decoder f_d using element-wise product between head embedding $\boldsymbol{z}_h$, relational embedding $\boldsymbol{r}_\tau$ and the tail embedding $\boldsymbol{z}_t$

$$f_d\left(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t\right) = \sum_{i=1}^{d} [\boldsymbol{z}_h]_i [\boldsymbol{r}_\tau]_i [\boldsymbol{z}_t]_i$$

  where $\boldsymbol{z}_h, \boldsymbol{z}_t, \boldsymbol{r}_\tau \in \mathbb{R}^d$.

- This type of decoder is a generalization of the dot-product decoders.

DistMult: Relational Patterns

- **Symmetry:**

$$f_d(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t) = \sum_{i=1}^{d} [\boldsymbol{z}_h]_i [\boldsymbol{r}_\tau]_i [\boldsymbol{z}_t]_i$$
$$= \sum_{i=1}^{d} [\boldsymbol{z}_t]_i [\boldsymbol{r}_\tau]_i [\boldsymbol{z}_h]_i$$
$$= f_d(\boldsymbol{z}_t, \tau, \boldsymbol{z}_h)$$

Therefore,

$$(v_h, \tau, v_t) \in E \iff (v_t, \tau, v_h) \in E$$

- **Anti-Symmetry:**

  - Since f_d is commutative, DistMult can model symmetric relational patters, but **not** anti-symmetric patterns.

DistMult: Relational Patterns

- **Inverse:**
  - For two node embeddings with inverse relations,

$$\sum_{i=1}^{d} [\boldsymbol{z}_h]_i \, [\boldsymbol{r}_{\tau_1}]_i \, [\boldsymbol{z}_t]_i = \sum_{i=1}^{d} [\boldsymbol{z}_t]_i \, [\boldsymbol{r}_{\tau_2}]_i \, [\boldsymbol{z}_h]_i$$

    Therefore, we conclude that

$$\boldsymbol{r}_{\tau_1} = \boldsymbol{r}_{\tau_2}$$

  - This is not acceptable as two different relations are represented with the same embedding.

ComplEx

- ComplEx approach improves DistMult by generalizing entity and relational embeddings to the **complex domain**.
- The ComplEx model is formulated as

$$f_d\left(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t\right) = \mathrm{Re}\left(\sum_{i=1}^{d} [\boldsymbol{z}_h]_i [\boldsymbol{r}_\tau]_i [\bar{\boldsymbol{z}}_t]_i\right)$$

  where $\boldsymbol{z}_h, \boldsymbol{r}_\tau, \boldsymbol{z}_t \in \mathbb{C}^d$ and $\bar{\boldsymbol{z}}_t$represent the complex conjugate of $\boldsymbol{z}_t$.
- Using the **complex conjugate** for entity v_t facilities modeling **asymmetric** relations.

ComplEx: Relational Patterns

- Symmetry:

$$d_f(\boldsymbol{z}_h, \tau, \boldsymbol{z}_t) = \text{Re}\left(\sum_{i=1}^{d} [\boldsymbol{z}_h]_i [\boldsymbol{r}_\tau]_i [\bar{\boldsymbol{z}}_t]_i\right)$$

$$= \sum_{i=1}^{d} \text{Re}\left([\boldsymbol{z}_h]_i [\boldsymbol{r}_\tau]_i [\bar{\boldsymbol{z}}_t]_i\right)$$

- If $Im(\boldsymbol{r}_\tau) = 0$, then

$$= \sum_{i=1}^{d} [\boldsymbol{r}_\tau]_i \text{Re}\left([\boldsymbol{z}_h]_i [\bar{\boldsymbol{z}}_t]_i\right)$$

$$= \sum_{i=1}^{d} [\boldsymbol{r}_\tau]_i \text{Re}\left([\bar{\boldsymbol{z}}_h]_i [\boldsymbol{z}_t]_i\right)$$

$$= \text{Re}\left(\sum_{i=1}^{d} [\boldsymbol{z}_t]_i [\boldsymbol{r}_\tau]_i [\bar{\boldsymbol{z}}_h]_i\right)$$

$$= d_f(\boldsymbol{z}_t, \tau, \boldsymbol{z}_h)$$

ComplEx: Relational Patterns

- **Inverse:**
- By setting

$$r_{\tau_1} = \bar{r}_{\tau_2}$$

It can represent inverse relations

- **Compositionality:**
- It can't represent compositional relations

Summary

- Knowledge graphs
- Knowledge graph Completion
- Multi-relational decoders
  - TransE
  - TransR
  - RotatE
  - RESCAL
  - DistMult
  - ComplEx