DSC250: Advanced Data Mining

Knowledge Graphs (KGs)

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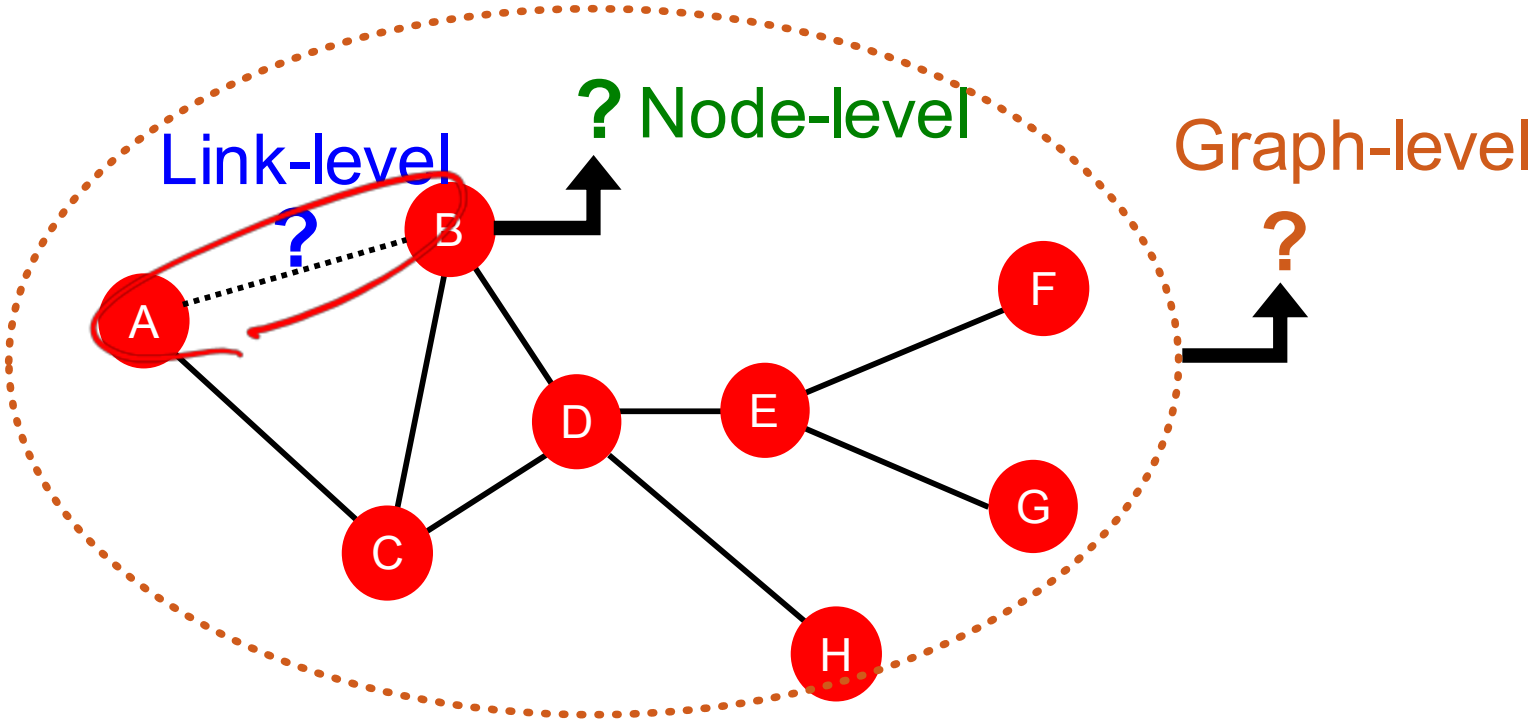
Outline

- Knowledge graphs

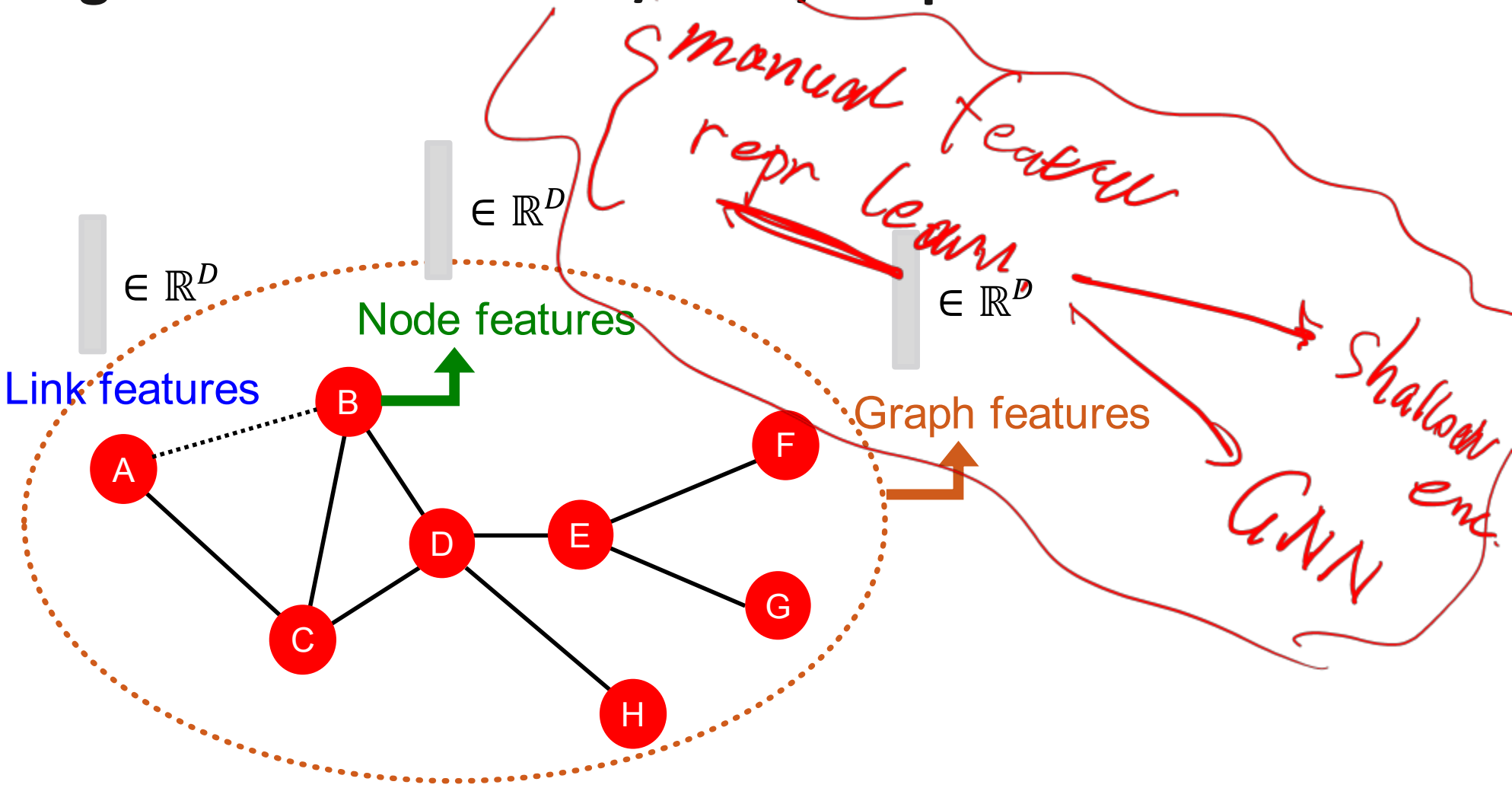
- Presentation
  - Lingyi Yang, Jiayue Yuan: "Generative Agents: Interactive Simulacra of Human Behavior"
  - Yuyuan Wu, Zijie Feng: "Data-efficient Fine-tuning for LLM-based Recommendation"
  - Ivy Nguyen, Joshua Chuang: "Prediction of COVID-19 cases by multifactor driven long short-term memory (LSTM) model"
  - Shuyu Wang, Caroline Zhang: "Yo'LLaVA: Your Personalized Language and Vision Assistant"

Recap: Tasks on Graph

- Node-level prediction
- Link-level prediction
- Graph-level prediction



Recap: Getting Features for Nodes/Links/Graphs

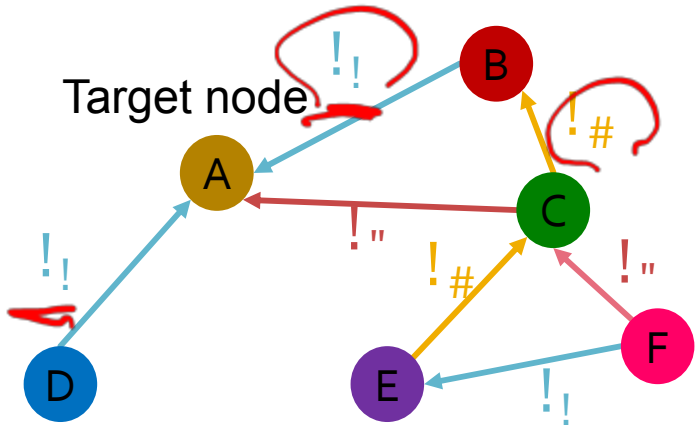


Outline

- Overview
- Knowledge Graph Completion (Link Prediction)
- Reasoning on Knowledge Graphs

Heterogeneous Graphs

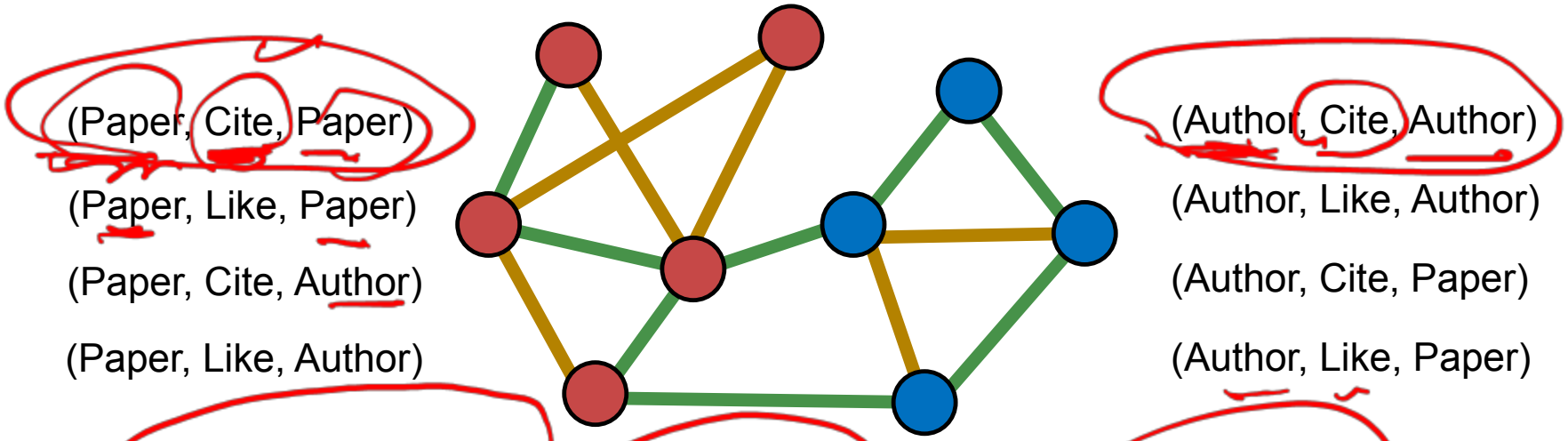
- **Heterogeneous graphs: a graph with multiple relation types**



Input graph

Heterogeneous Graphs

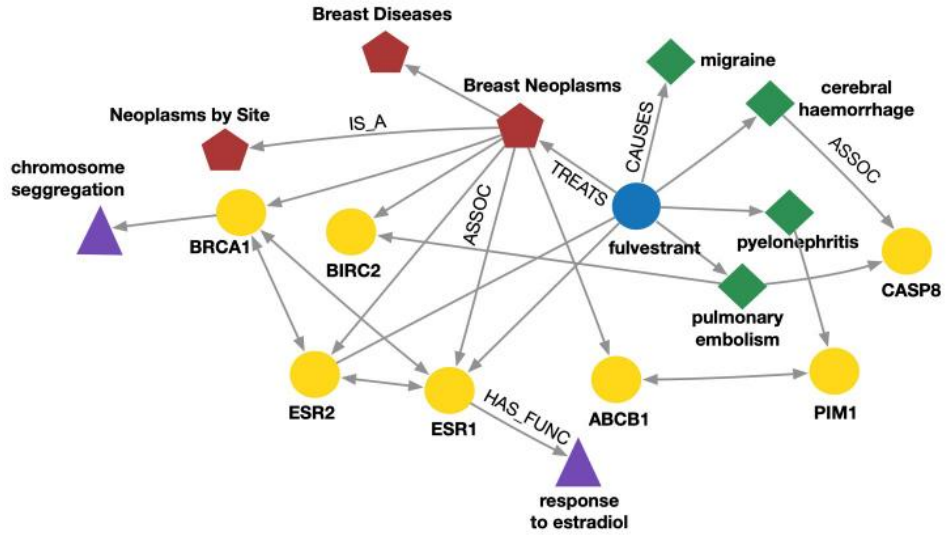
8 possible relation types!

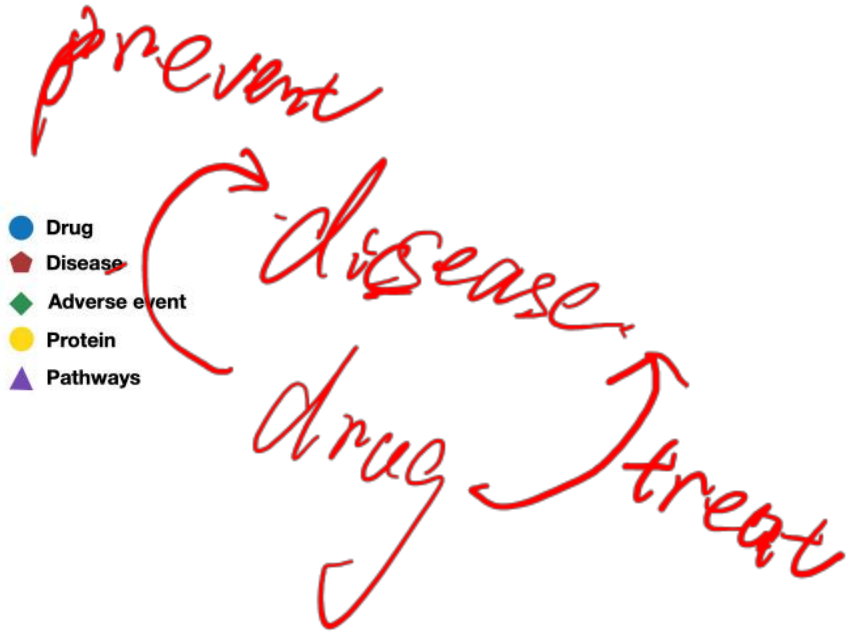


Relation types: (node_start, edge, node_end)

- We use **relation type to describe an edge** (as opposed to edge type)
- Relation type better captures the interaction between nodes and edges

Heterogeneous Graphs





Biomedical Knowledge Graphs

Example node: Migraine

Example relation: (fulvestrant, Treats, Breast Neoplasms)

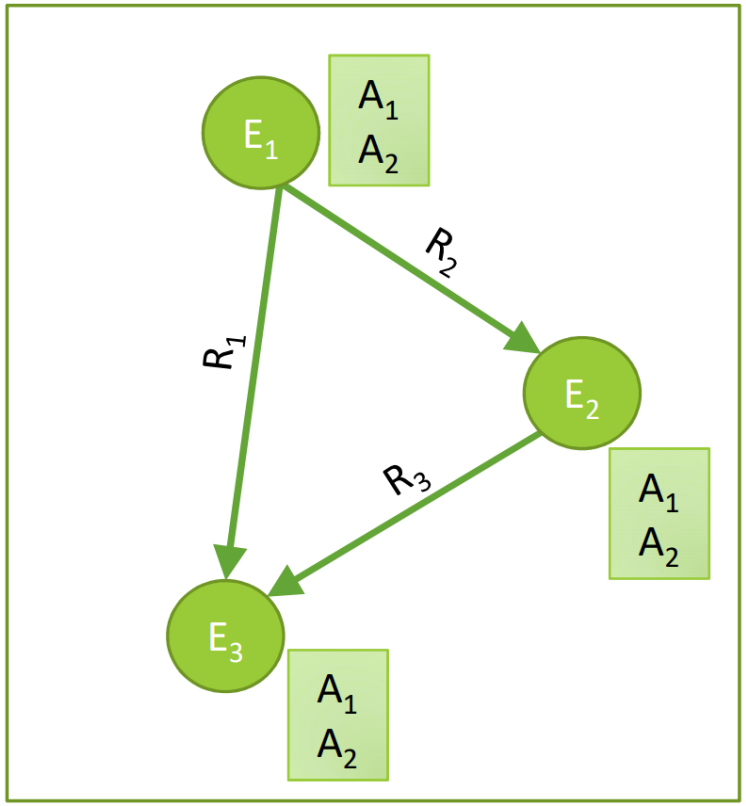
Example node type: Protein

Example edge type: Causes

Knowledge Graph

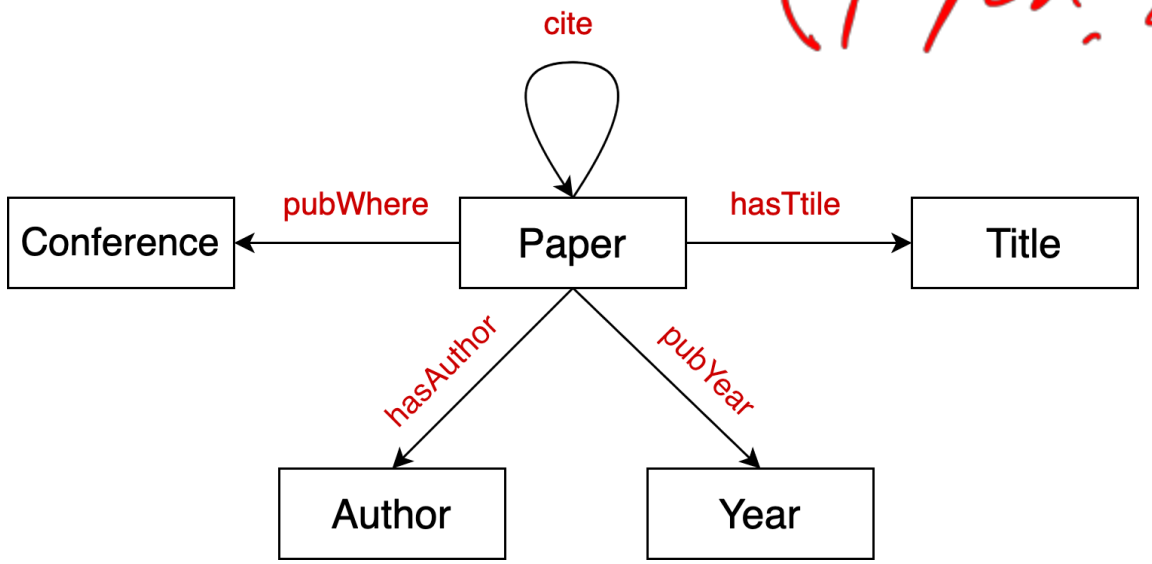
Knowledge in graph form:

- § 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**



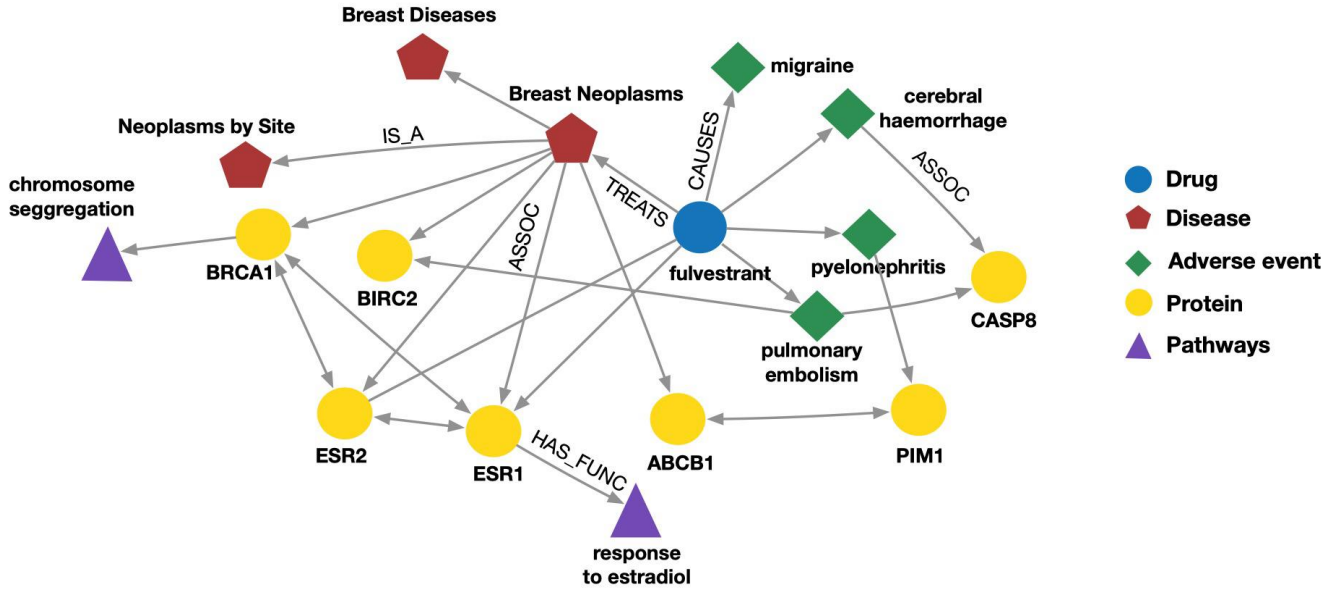
Example: Bibliographic Networks

- **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



KGs 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 KGs

- **Serving information:**

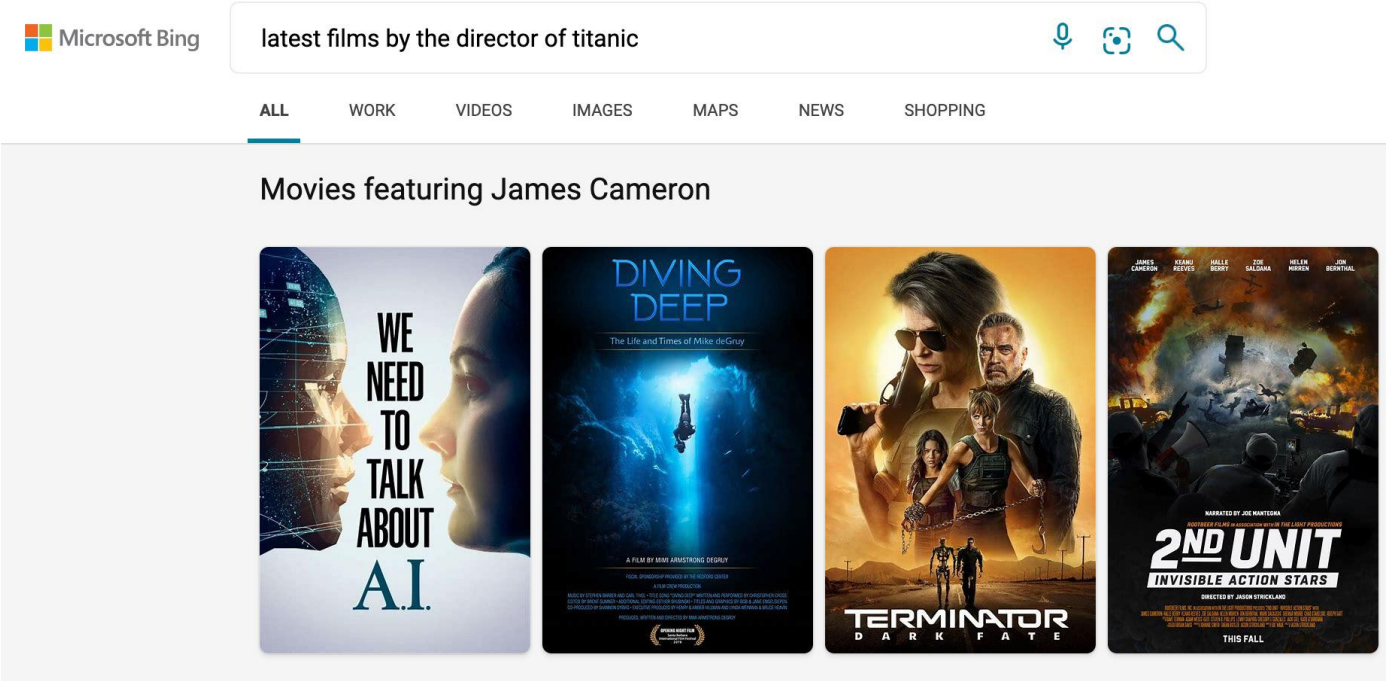


Image credit: Bing

Applications of KGs

- **Question answering and conversation agents**

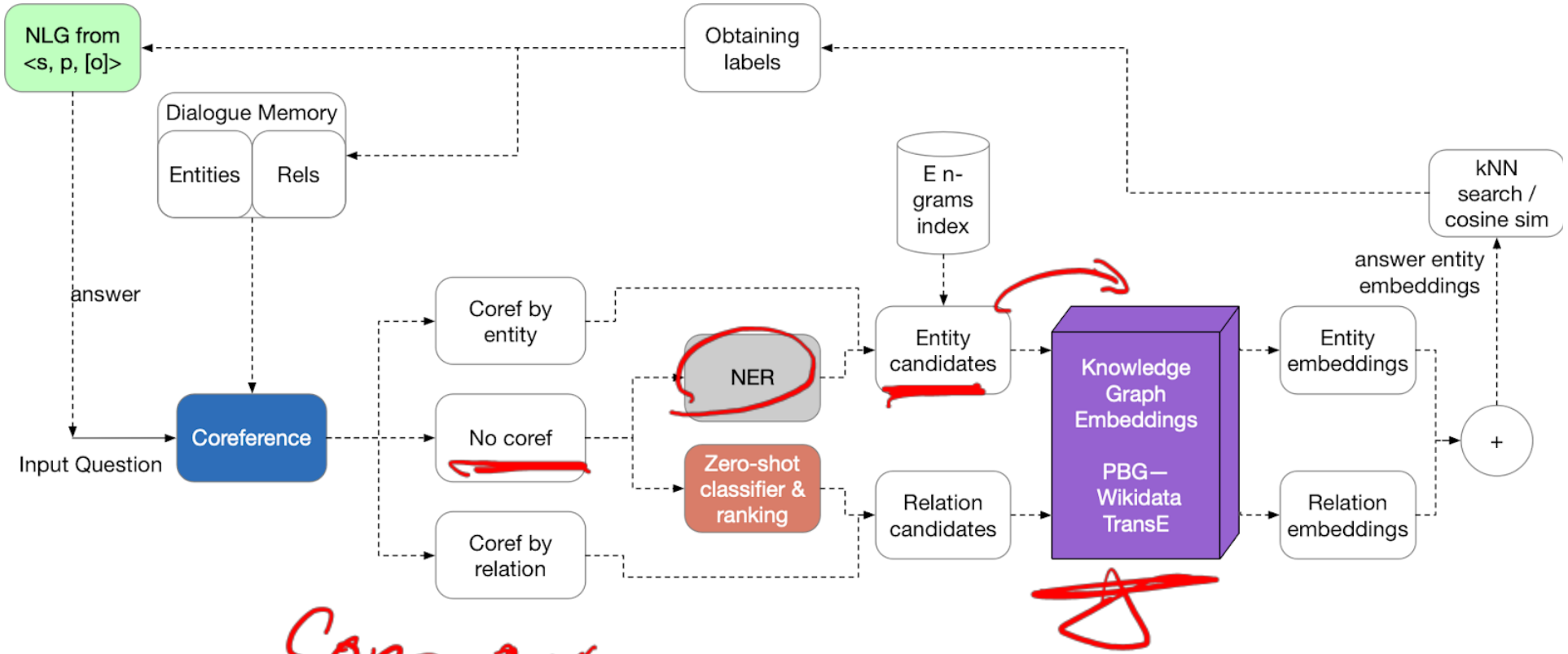


Image credit: Medium

KG Datasets

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

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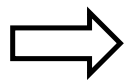
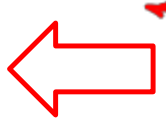
Given a massive KG, enumerating all the possible facts is intractable!



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.

Outline

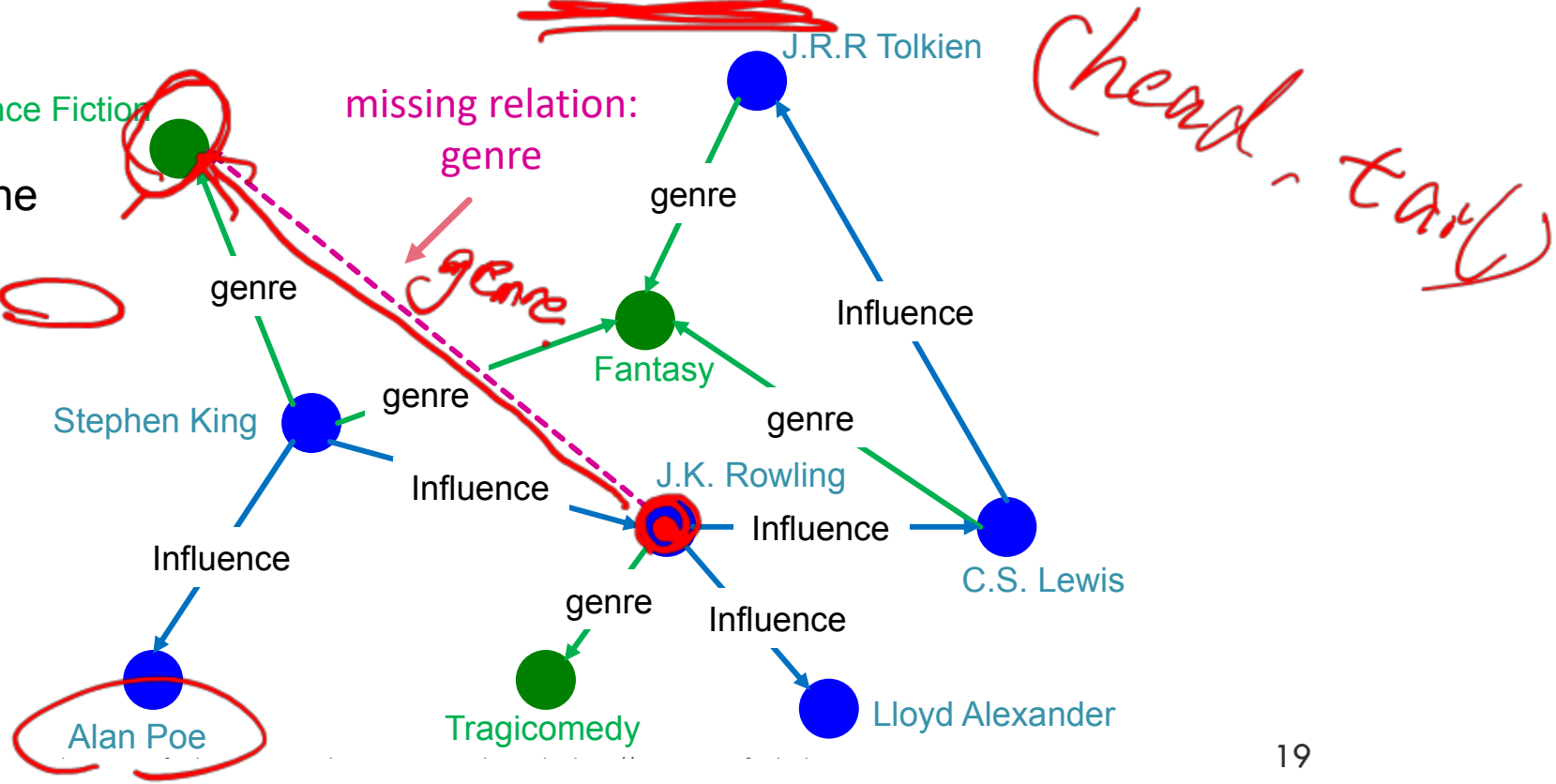
- Overview
- **Knowledge Graph Completion (Link Prediction)**
- Reasoning on Knowledge Graphs

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")



KG Representation

- Edges in KG are represented as **triples** $(h, \$, \%)$
  - head (h) has relation $(\$)$ with tail $(\%)$

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- **Key Idea:**
  - Model entities and relations in embedding space $\mathbb{R}^d$
    - Associate entities and relations with **shallow embeddings**
      - **Note we do not learn a GNN here!**

KG Representation

- Edges in KG are represented as **triples** $(h, \$, \%)$
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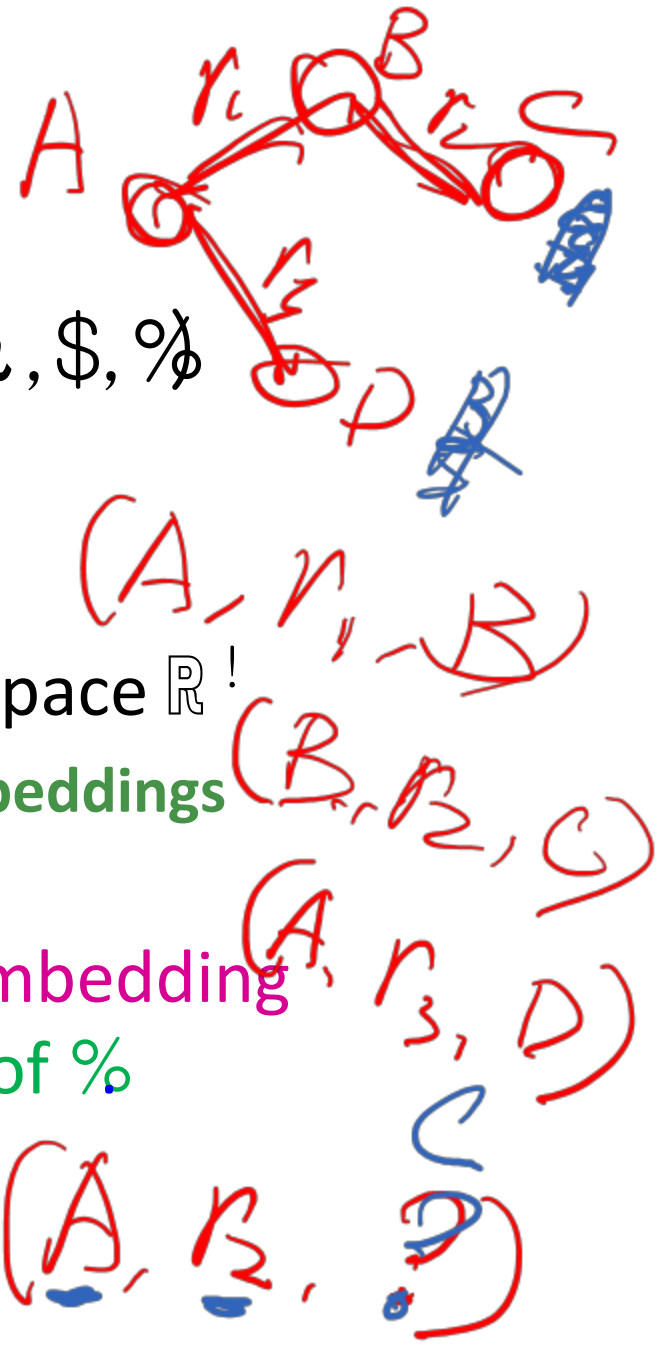
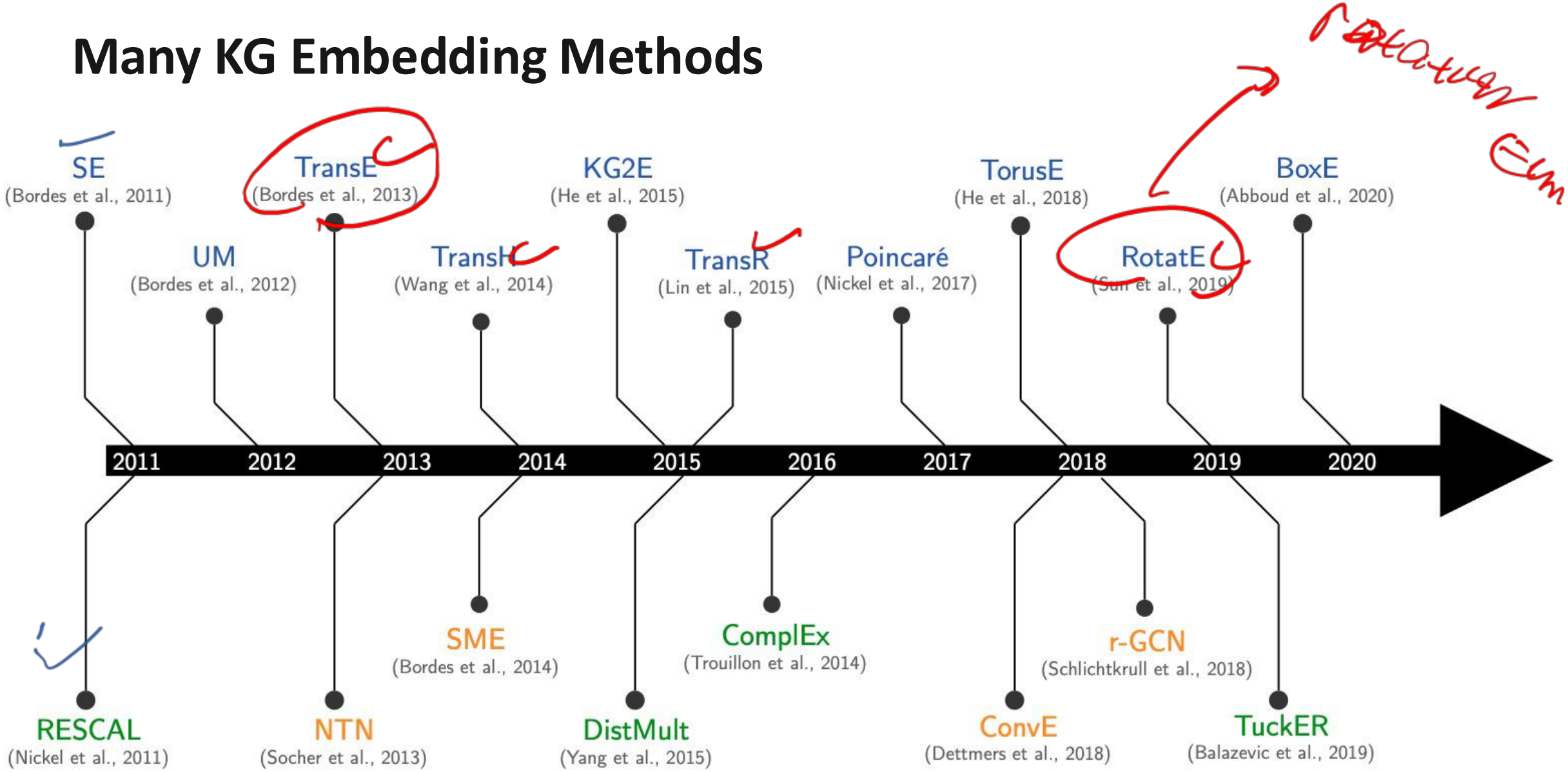
- **Key Idea:**
  - Model entities and relations in embedding space $\mathbb{R}^!$
    - Associate entities and relations with **shallow embeddings**
      - **Note we do not learn a GNN here!**
  - Given a triple $(h, \$, \%)$, the goal is that the embedding of $(h, \$)$ **should be close** to the embedding of $\%$
    - How to embed $(h, \#)$?
    - How to define score $\$(h, \%)$?
      - Score $"_!$ is high if $(h, \&, ')$ exists, else $"_!$ is low



Many KG Embedding Methods



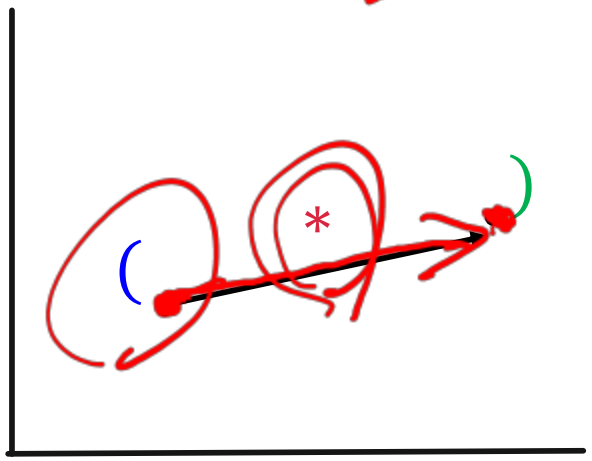
TransE for KG Completion

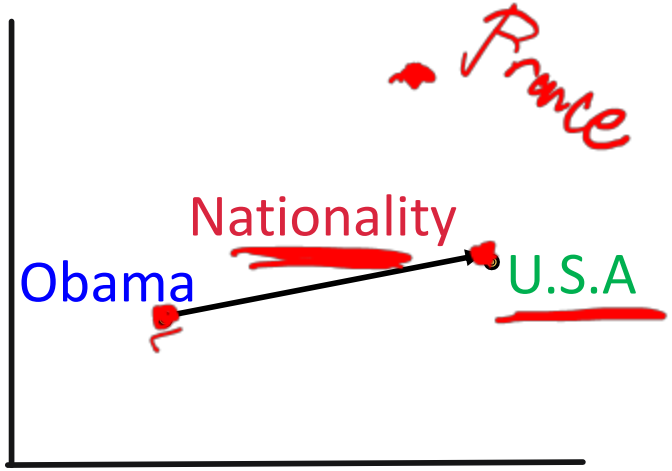
- **Intuition: Translation**

  For a triple (h, r, t), let $\mathbf{h}, \mathbf{r}, \mathbf{t} \in \mathbb{R}^!$ be embedding vectors.

  embedding vectors will appear in boldface

- **TransE:** $\mathbf{h} + \mathbf{r} \approx \mathbf{t}$ if the given link exists else $\mathbf{h} + \mathbf{r} \neq \mathbf{t}$





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

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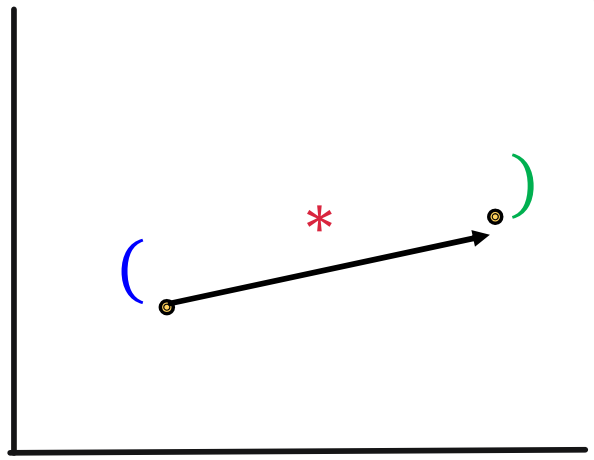
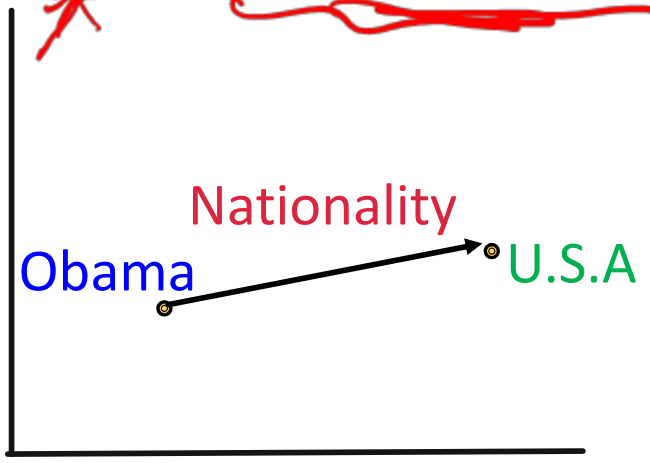
Entity scoring function: $f_r(h, t) = -||\mathbf{h} + \mathbf{r} - \mathbf{t}||$





$f_r(h, t_1)$

$f_r(h, t_2)$

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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.

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    - **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?**

Four Relationship 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: Hypernym (a word with a broader meaning: poodle vs. dog)
- **Inverse Relations:**

$$r_{(}(h,t) \Rightarrow r_{)}(t,h)$$

  - **Example** : (Advisor, Advisee)
- **Composition (Transitive) Relations:**

$$r_{)}(x,y) \wedge r_{(}(y,z) \Rightarrow r_{*}(x,z) \quad \forall x,y,z$$

  - **Example**: My mother's husband is my father.
- **1-to-N relations:**

$$r(h,t_{)}), r(h,t_{(}), \ldots, r(h,t_{+}) \text{ are all True.}$$

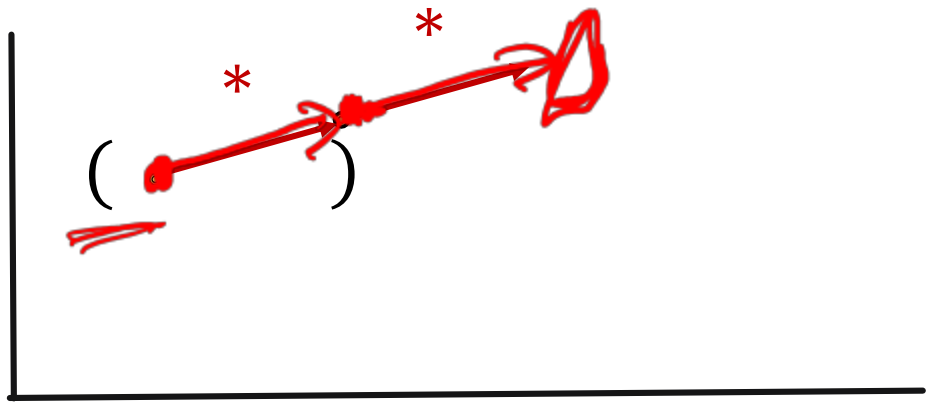
  - **Example**: # is "StudentsOf"

Antisymmetric Relations in TransE

- **Antisymmetric Relations:**

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

  - **Example**: Hypernym (a word with a broader meaning: poodle vs. dog)
- **TransE** can model antisymmetric relations ü
  - $(+ * =)$, but $) + * \neq ($

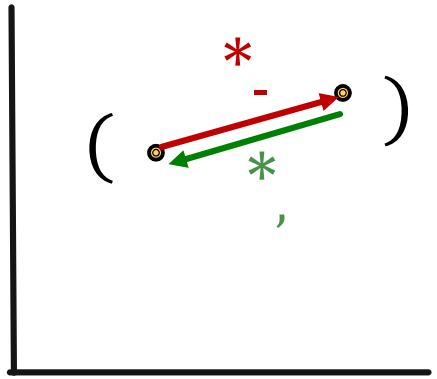


Inverse Relations in TransE

- **Inverse Relations:**

$$\$_{\#}(h, \%) \Rightarrow \$_{\$}(\%, h)$$

  - **Example** : (Advisor, Advisee)
- **TransE** can model inverse relations ü
  - ($+ *_{,} =$), we can set $*_{)} = -*_{(}$



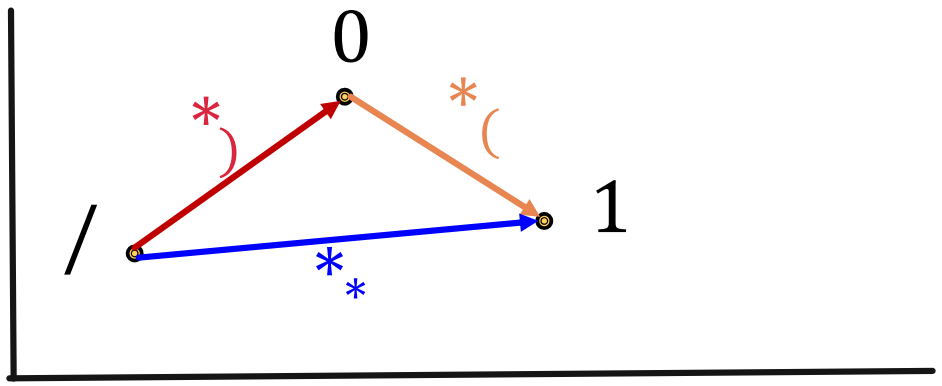
Composition in TransE

- **Composition (Transitive) Relations:**

$$\$_{\$}(7,8) \wedge \$_{\#}(8,:) \Rightarrow \$_{\%}(7,:) \quad \forall 7,8,:$$

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

$$(_{\%} = (_{\$} + (_{\#}$$



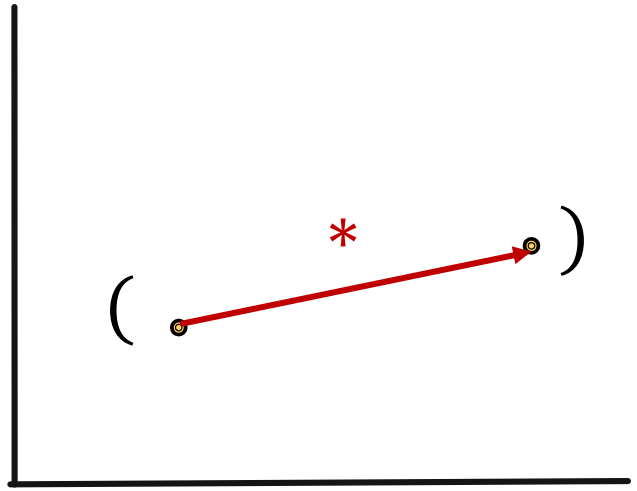
Limitations of TransE: Symmetric Relations

- **Symmetric Relations:**

$$\$(h, \%) \Rightarrow \$(\%, h) \square \forall h, \%$$

  - **Example**: Family, Roommate
- **TransE cannot** model symmetric relations û

only if (= 0, ' =)

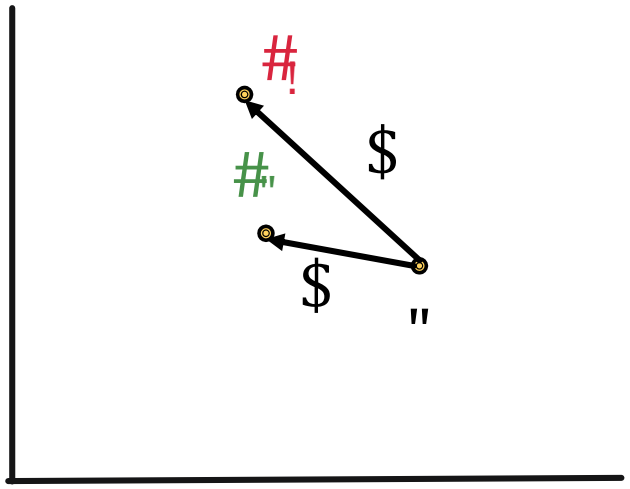


For all h, t that satisfy $r(h, t)$, $r(t, h)$ is also True, which means $\|\mathbf{h} + \mathbf{r} - \mathbf{t}\| = 0$ and $\|\mathbf{t} + \mathbf{r} - \mathbf{h}\| = 0$. Then $\mathbf{r} = 0$ and $\mathbf{h} = \mathbf{t}$, however h and t are two different entities and should be mapped to different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

Limitations of TransE: 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 û
  - $\mathbf{t}_1$ and $\mathbf{t}_2$ will map to the same vector, although they are different entities

- $)_{\$} = ' + (=)_{\#}$
- $)_{\$} \neq)_{\#}$ contradictory!



KG Completion Methods

Model	Score	Embedding	Sym.	Antisym.	Inv.	Compos.	1-to-N
TransE	$-\|\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|\|$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{R}^{!}$	û	ü	ü	ü	û
TransR	$-\|\|\boldsymbol{M}_{"}\mathbf{h}+\mathbf{r}-\boldsymbol{M}_{"}\mathbf{t}\|\|$	$\mathbf{h},\mathbf{t}\in\mathbb{R}^{!}$, $\mathbf{r}\in\mathbb{R}^{\#}$, $\boldsymbol{M}_{"}\in\mathbb{R}^{\#\times!}$	ü	ü	ü	ü	ü
DistMult	$<\mathbf{h},\mathbf{r},\mathbf{t}>$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{R}^{!}$	ü	û	û	û	ü
ComplEx	$\mathrm{Re}(<\mathbf{h},\mathbf{r},\bar{\mathbf{t}}>)$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{C}^{!}$	ü	ü	ü	û	ü
RotateE	$-\|\|\mathbf{h}\circ\mathbf{r}-t\|\|$	$\mathbf{h},\mathbf{t},\mathbf{r}\in\mathbb{C}^{!}$	ü	ü	ü	ü	ü

Questions?