大模型时代下的知识图谱归纳式推理

Rethinking Inductive KG Reasoning with Language Models

杭州电子科技大学 · 耿玉霞 · 2023.10.22

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02 知识图谱归纳式推理

03 知识图谱推理与大模型

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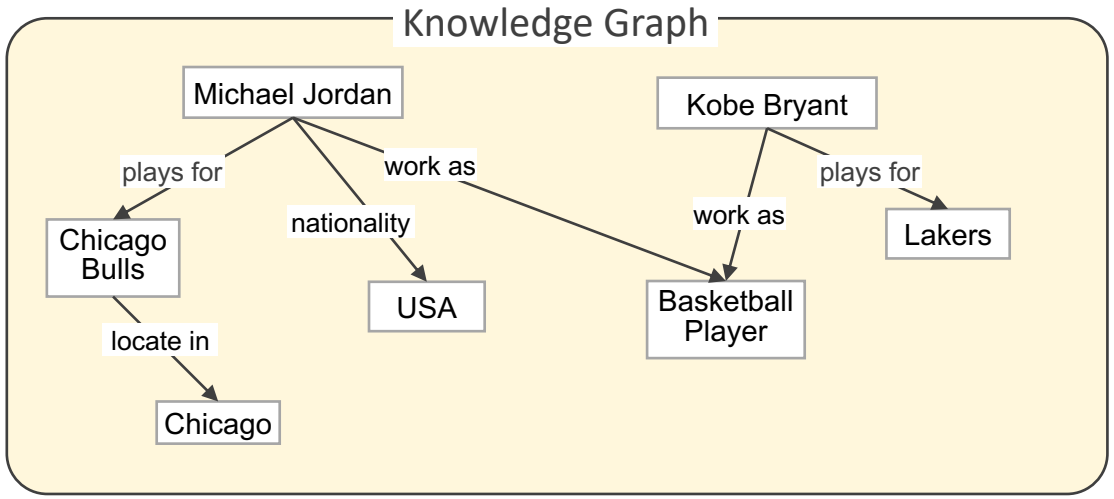
➢ 知识图谱推理

- ➢ 基于已知的三元组事实，推理出新的、未知的事实、关系、范式(Axioms)、规则(Rules)

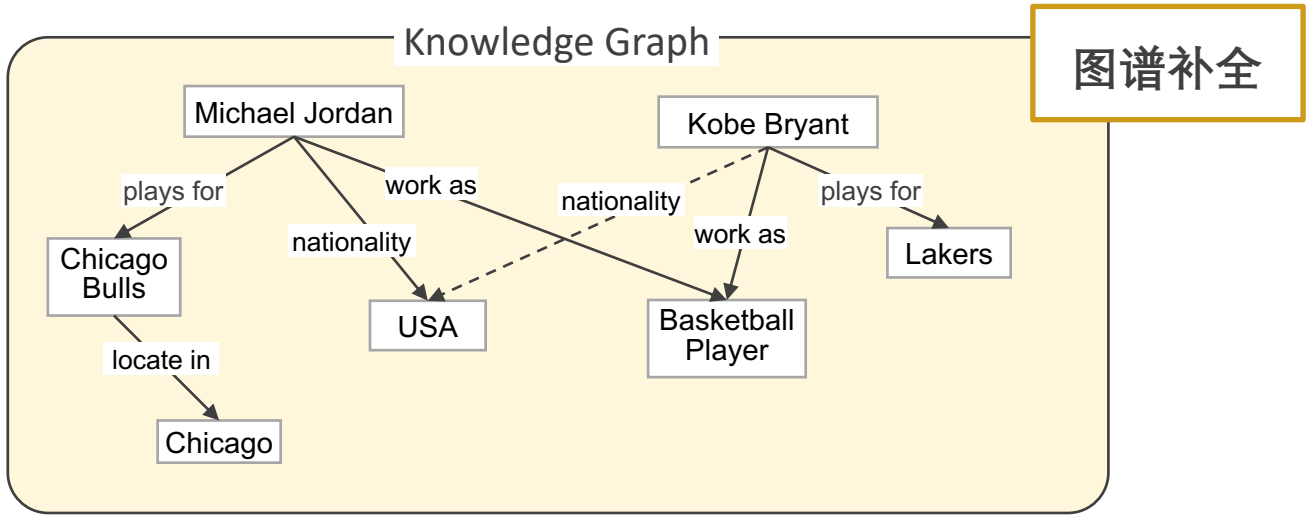


新事实
新关系
新范式
新规则

属性补全
关系预测
错误检测
问句扩展
语义理解

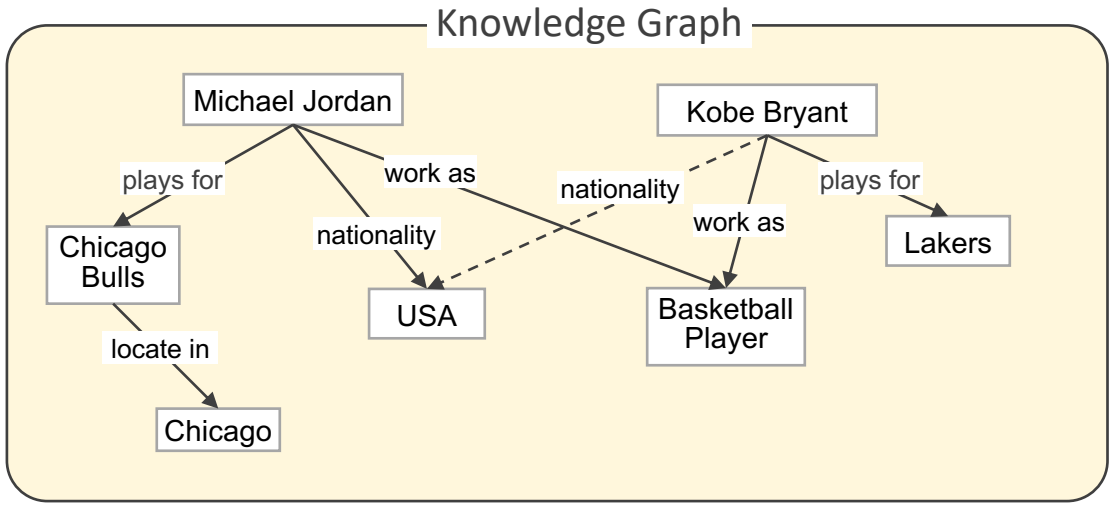
- **知识图谱推理**
  - 基于已知的三元组事实，推理出新的、未知的事实、关系、范式(Axioms)、规则(Rules)
- **基于向量表示的知识图谱推理技术**
  - 为知识图谱中的每个实体和关系都学习一个向量表示，同时保留图谱中的结构信息和语义信息；
  - 将离散的符号表示转换为连续的向量表示，对接各种下游任务，特别是**推理任务**；
  - 将推理转换为向量或矩阵之间的计算过程，提升大规模图谱推理效率。

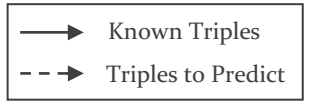
KG Embeddings = Entity Vector & Relation Vectors = Distributed Representations of Knowledge Graph



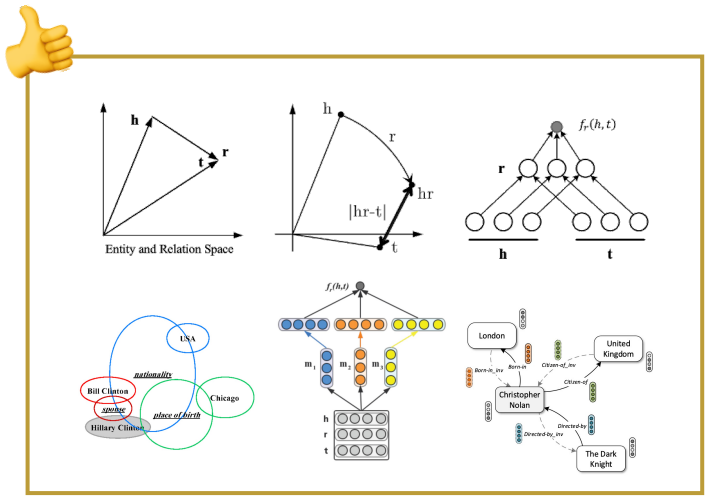
知识图谱推理补全

➢ 传统补全模式及典型算法





1. 训练阶段：学习实体和关系的表示
2. 直推式推理：测试实体和关系都被训练过

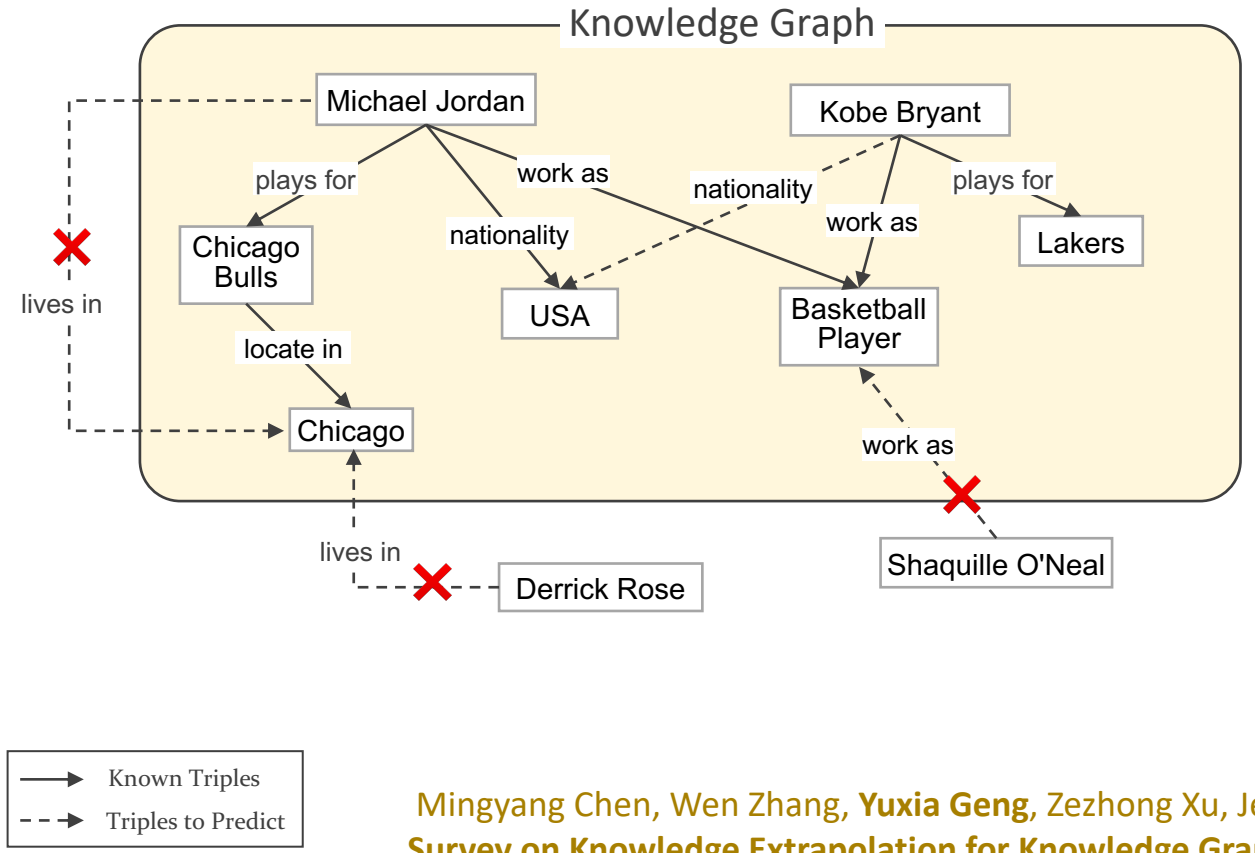


TransE, DistMult, RotatE, R-GCN, CompGCN, …

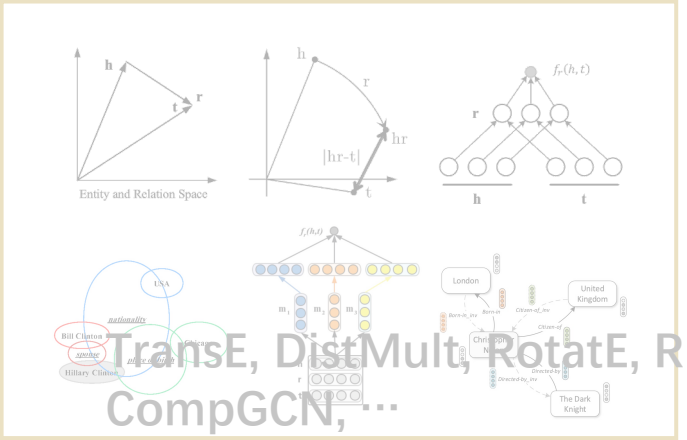
Wang, Quan, et al. "Knowledge graph embedding: A survey of approaches and applications." TKDE 2017.

知识图谱推理补全

➢ 新的补全模式



1. 训练阶段：学习实体和关系的表示
2. 直推式推理：测试实体和关系都被训练过
3. 归纳式推理1：测试时新实体，向量未知
4. 归纳式推理2：测试时新关系，向量未知
5. 归纳式推理3：测试时新实体+新关系，向量未知



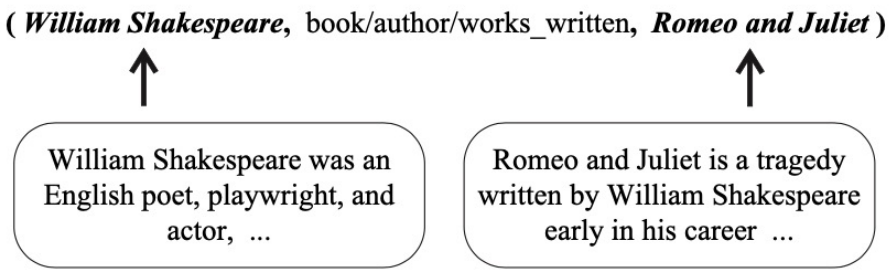
Mingyang Chen, Wen Zhang, **Yuxia Geng**, Zezhong Xu, Jeff Z Pan, Huajun Chen. **Generalizing to Unseen Elements: A Survey on Knowledge Extrapolation for Knowledge Graphs**. IJCAI 2023.
Jiaoyan Chen, **Yuxia Geng**, Zhuo Chen, Jeff Z. Pan, Yuan He, Wen Zhang, Ian Horrocks, Huajun Chen. **Zero-shot and Few-shot Learning with Knowledge Graphs: A Comprehensive Survey**. Proceedings of the IEEE 2023.

知识图谱归纳式推理：外源信息辅助

- **基于外源信息学习新实体/新关系的向量表示**
  - 实体关系的文本、实体的图像
  - 知识图谱本体
  - 额外提供的辅助三元组
    - 辅助三元组，用于建立新旧实体之间的关联，**图神经网络**
    - 辅助三元组，用于建立推理所需的上下文**子图**结构，**图神经网络**
    - 少量辅助三元组，少量推理样本，**元学习**
  - **全归纳式 & 半归纳式**
  - **零样本 & 少样本**

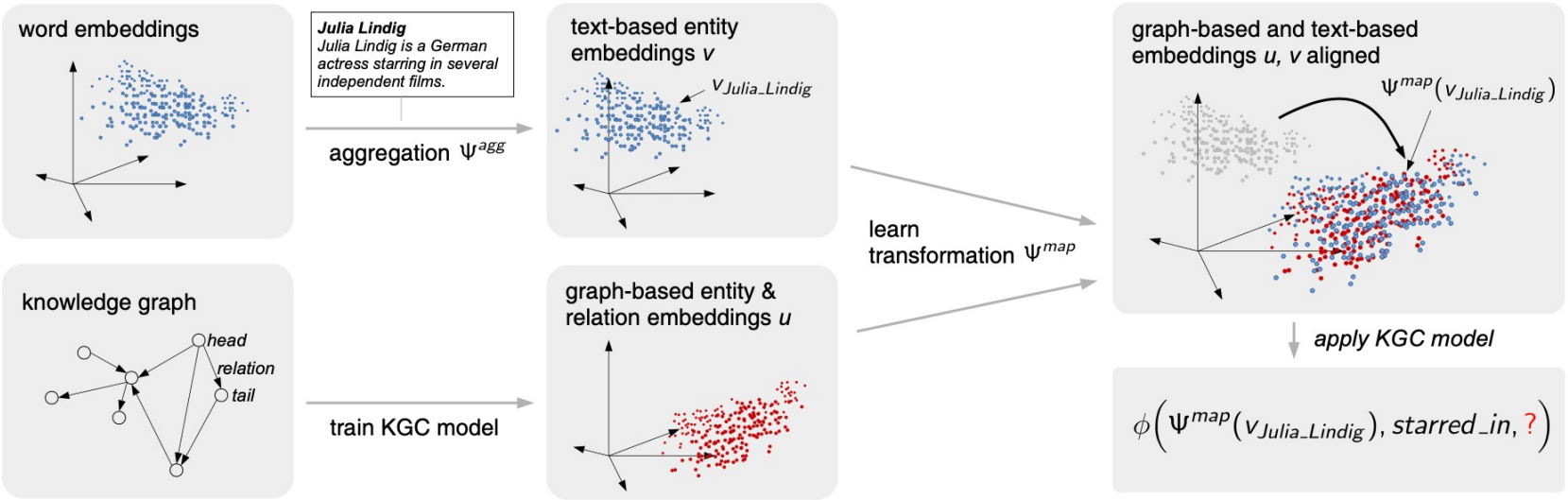
新实体：文本或图像

➢ 基于实体的文本描述或图像，表示新实体



Xie, Ruobing, et al. "**DKRL**: Representation learning of knowledge graphs with entity descriptions." AAAI 2016.

Xie, Ruobing, et al. "**IKRL:** Image-embodied knowledge representation learning." IJCAI 2017.



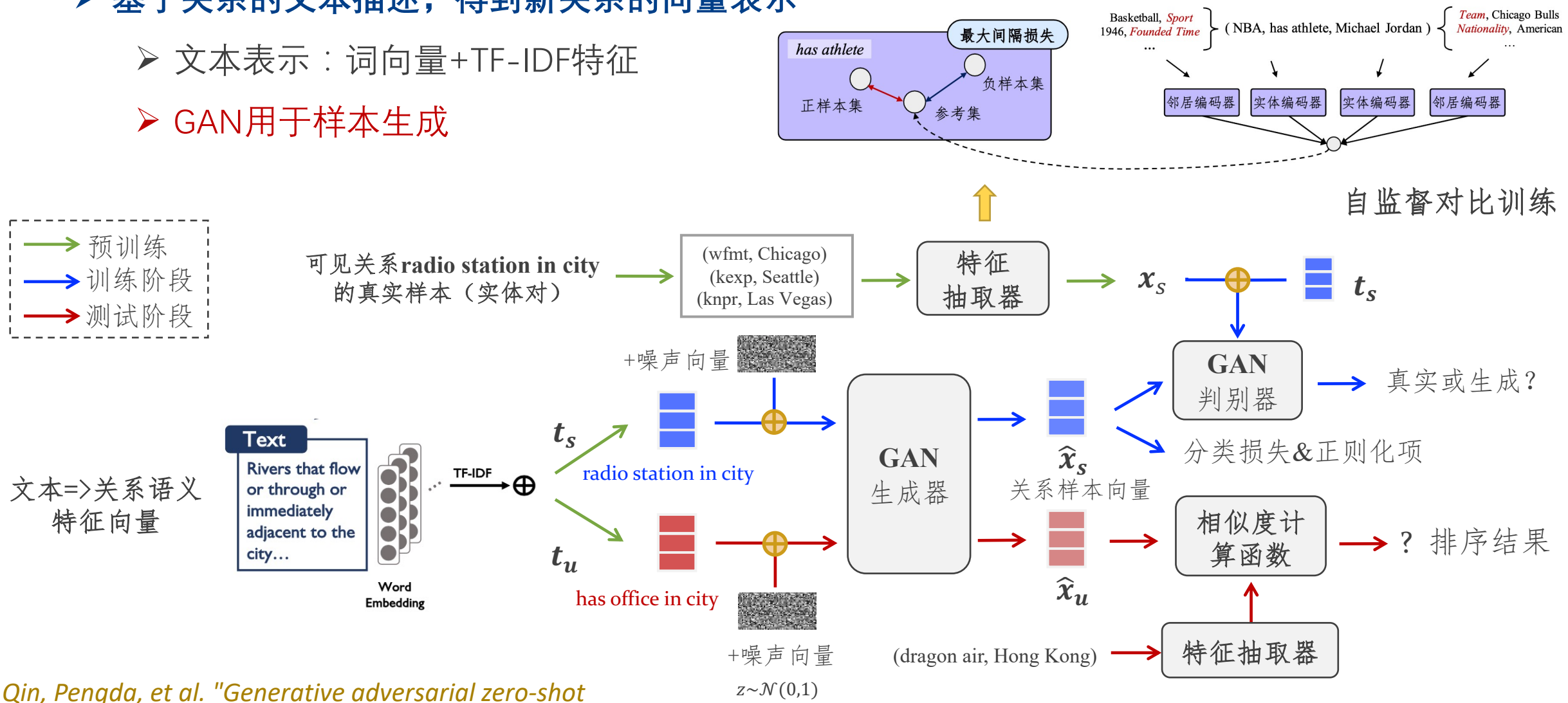
Shah, Haseeb, et al. "**OWE**: An open-world extension to knowledge graph completion models." AAAI 2019.

$$v_h := \Psi^{agg}\left(v_{w_1}, v_{w_2}, \ldots, v_{w_n}\right)$$

$$score(h,r,t) = \phi\left(\Psi^{map}(v_h), u_r, u_t\right)$$

新关系：文本

- 基于关系的文本描述，得到新关系的向量表示
  - 文本表示：词向量+TF-IDF特征
  - GAN用于样本生成



Qin, Pengda, et al. "Generative adversarial zero-shot relational learning for knowledge graphs." AAI 2020.

新关系：本体

➢ 知识图谱本体为实体和关系定义了更丰富的语义关系

Textual Descriptions

radionstationincity: specifies that a particular radio station is headquarted in a particular city

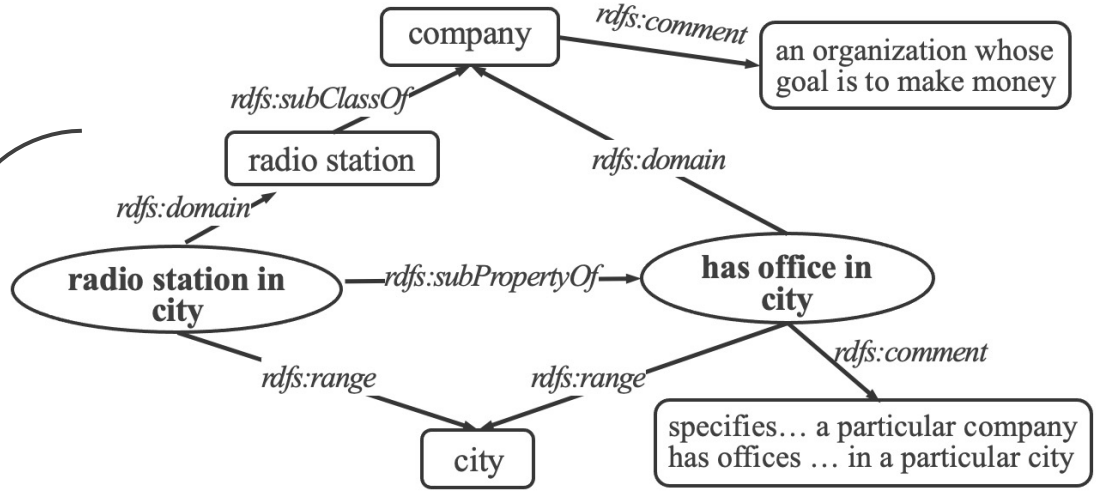
hasofficeincity: specifies that a particular company has offices in a particular city

Seen KG Relation:
radio_station_in_city

特征迁移

Unseen KG Relation:
has_office_in_city

Ontological Schema



The Ontological Schemas contains different kinds of relation knowledge including textual names and descriptions, and relation semantics from RDFS and OWL.

Yuxia Geng, Jiaoyan Chen, Zhuo Chen, Jeff Z. Pan, Zhiquan Ye, Zonggang Yuan, Yantao Jia, and Huajun Chen. **OntoZSL: Ontology-enhanced zero-shot learning**. WWW 2021.
Yuxia Geng, Jiaoyan Chen, Wen Zhang, Yajing Xu, Zhuo Chen, Jeff Z. Pan,Yufeng Huang, Feiyu Xiong, and Huajun Chen. **Disentangled Ontology Embedding for Zero-shot Learning**. KDD 2022.

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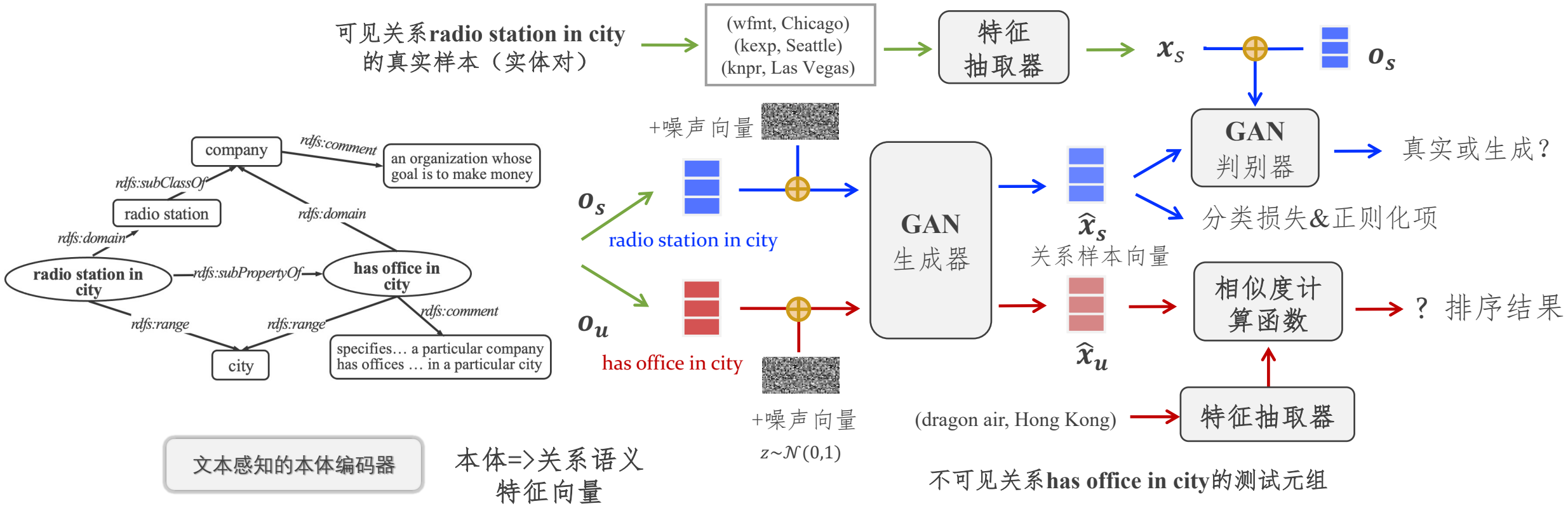

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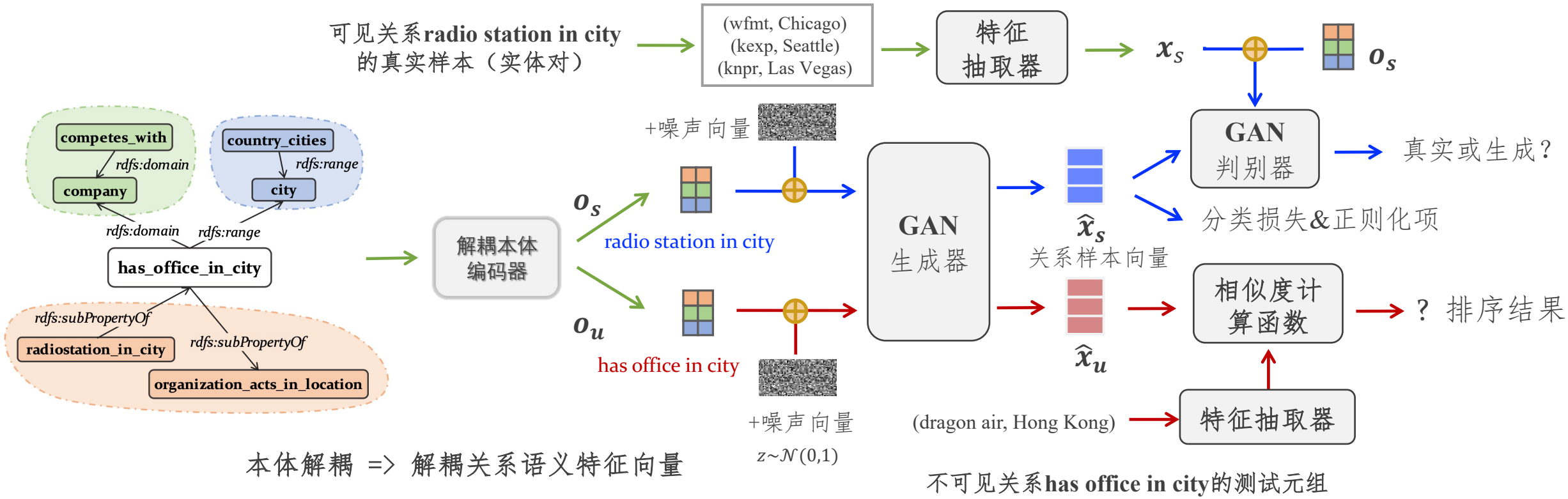

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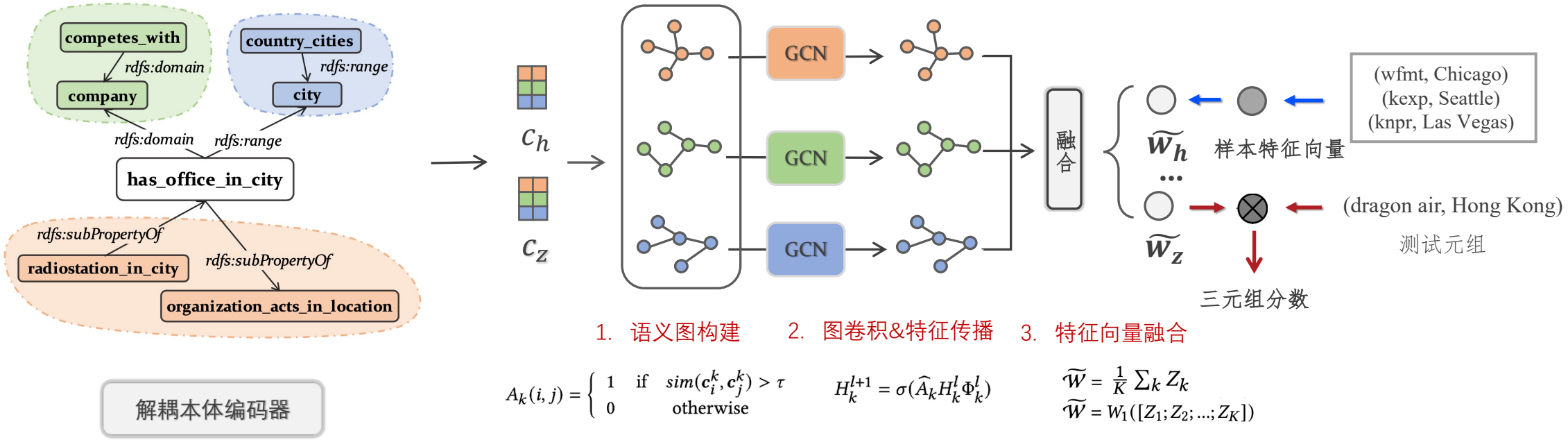


$$A_k(i,j) = \begin{cases} 1 & \text{if } sim(\mathbf{c}_i^k, \mathbf{c}_j^k) > \tau \\ 0 & \text{otherwise} \end{cases}$$

$$H_k^{l+1} = \sigma(\widehat{A}_k H_k^l \Phi_k^l)$$

$$\widetilde{W} = \frac{1}{K}\sum_k Z_k$$

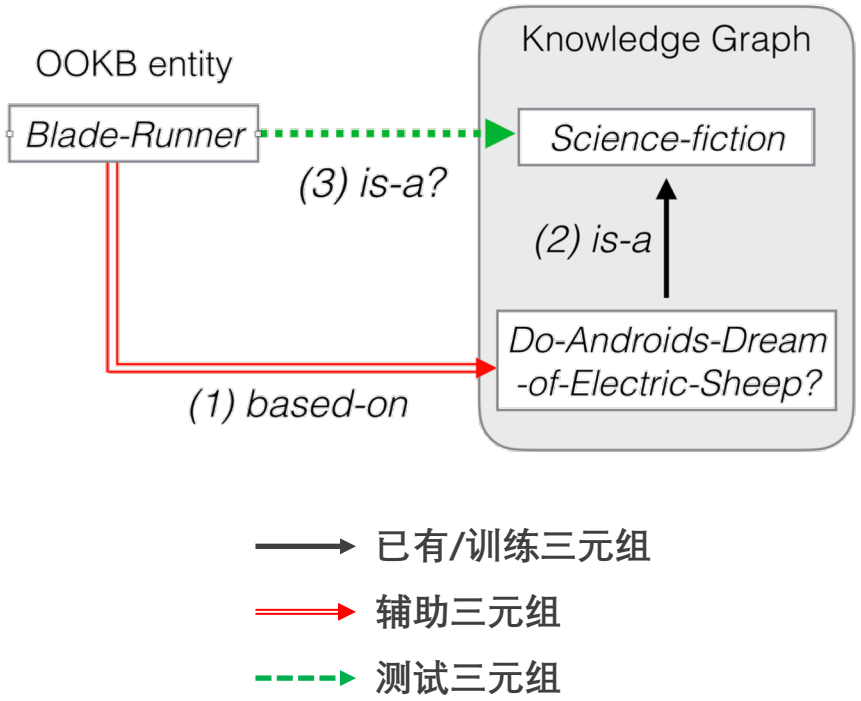
$$\widetilde{W} = W_1([Z_1; Z_2; \ldots; Z_K])$$

→ 训练阶段
→ 测试阶段

Yuxia Geng, Jiaoyan Chen, Wen Zhang, Yajing Xu, Zhuo Chen, Jeff Z. Pan,Yufeng Huang, Feiyu Xiong, and Huajun Chen. **Disentangled Ontology Embedding for Zero-shot Learning**. KDD 2022.

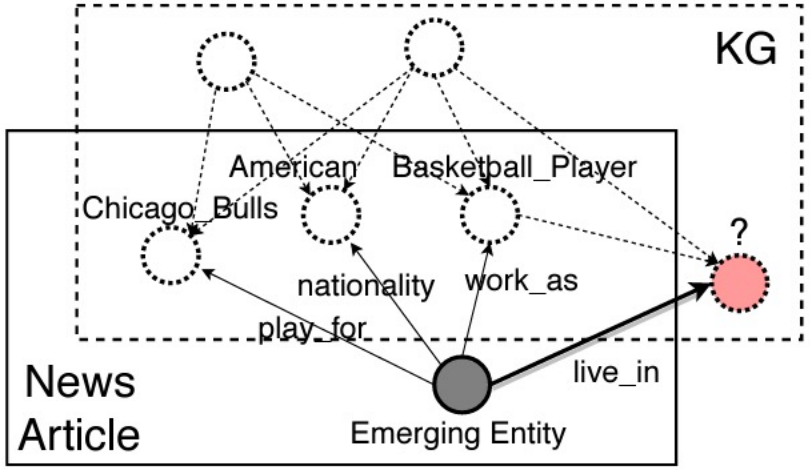
新实体：辅助三元组

- 测试时额外提供一些三元组，用于关联新实体与旧实体
  - OOKB entity: Out-of-Knowledge-Base entity



$$\mathbf{v}_e^{(n)} = \begin{cases} \mathbf{v}_e, & \text{if } n = 0, \\ P(S_{\text{head}}^{(n-1)}(e) \cup S_{\text{tail}}^{(n-1)}(e)), & \text{otherwise,} \end{cases}$$

$$S_{\text{head}}(e) = \{T_{\text{head}}(\mathbf{v}_h; h, r, e) \mid (h, r, e) \in \mathcal{N}_h(e)\},$$
$$S_{\text{tail}}(e) = \{T_{\text{tail}}(\mathbf{v}_t; e, r, t) \mid (e, r, t) \in \mathcal{N}_t(e)\},$$

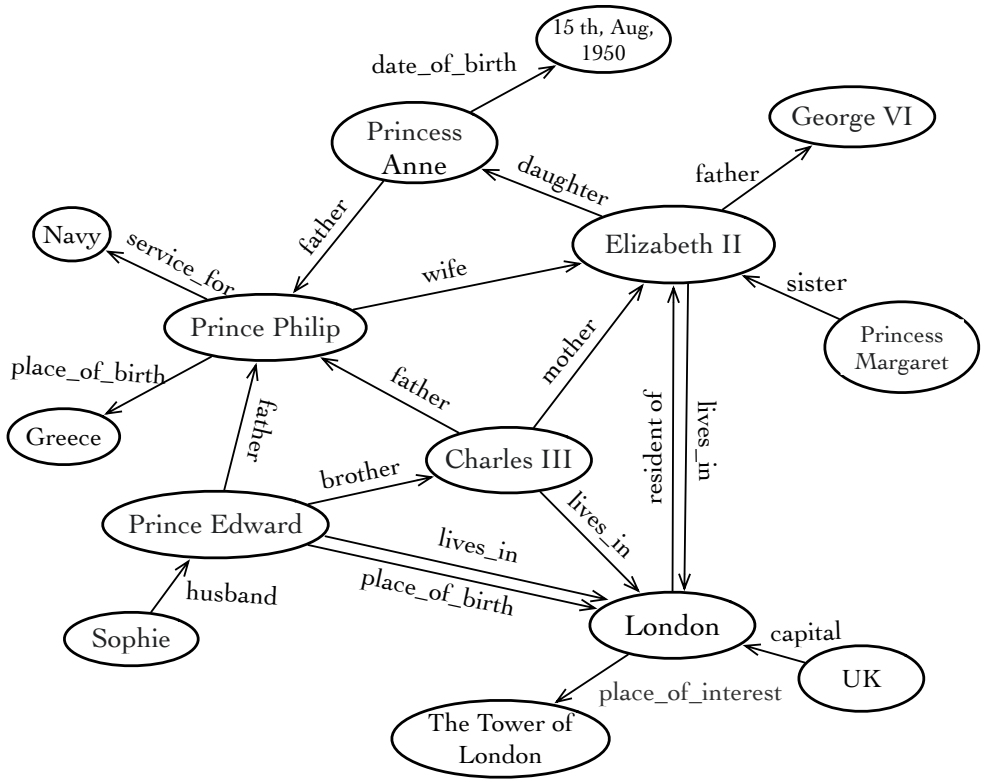


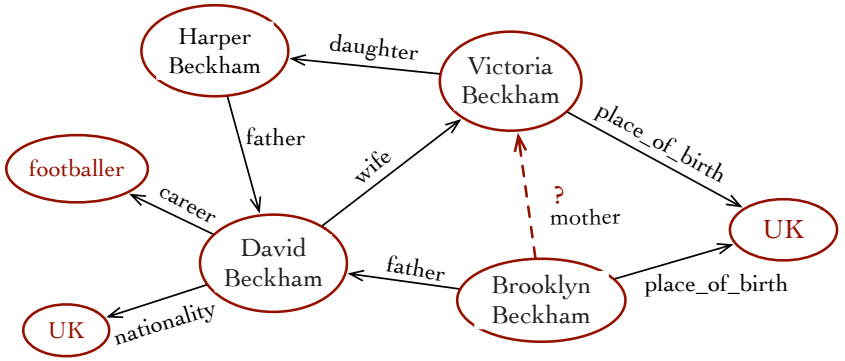
Hamaguchi, Takuo, et al. "Knowledge transfer for out-of-knowledge-base entities: A graph neural network approach." IJCAI 2017.

Wang, Peifeng, et al. ”**LAN:** Logic attention based neighborhood aggregation for inductive knowledge graph embedding." AAAI 2019.

新实体：辅助三元组营造推理上下文

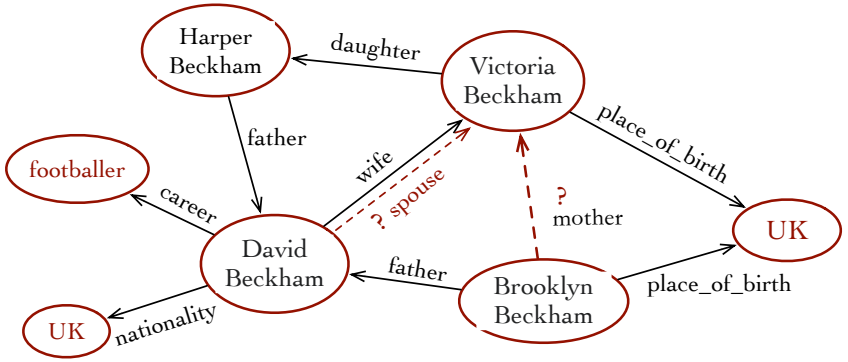
- 从三元组周围的局部子图中挖掘推理线索，如可迁移泛化的规则
  - 基于辅助三元组建立推理所需的上下文图结构
  - 可以处理全新的图谱





新图谱
实体全新

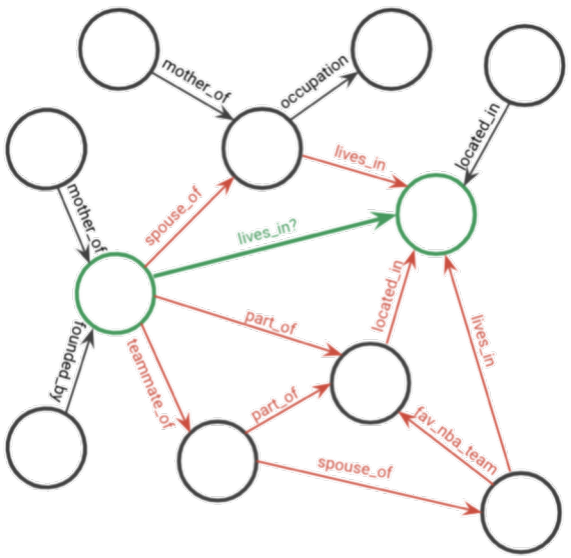
$$\exists Y.(X, father, Y) \wedge (Y, wife, Z) \Longrightarrow (X, mother, Z)$$



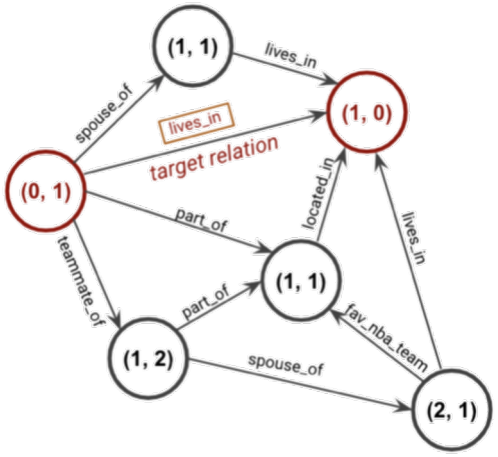
新图谱
实体全新
+新增关系

新实体：辅助三元组营造推理上下文

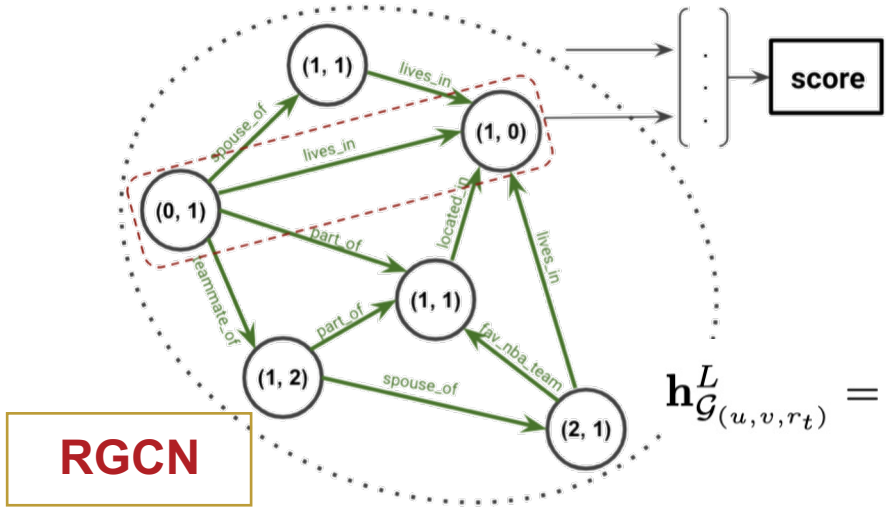
- 从三元组周围的局部子图中挖掘推理线索，如可迁移泛化的规则
  - GraIL：不为实体学习固定的向量表示，泛化至新实体



1. Sample the enclosing sub-graph around the link to be predicted (target link).



2. Label the nodes w.r.t the target nodes to identify their structural role. Uniquely labels target nodes to mark them for the model.



$$\mathbf{h}^L_{\mathcal{G}(u,v,r_t)} = \frac{1}{|\mathcal{V}|}\sum_{i\in\mathcal{V}} \mathbf{h}^L_i$$

3. Pass messages across the (sub-)graph to predict a score indicating how strongly the structure around the target link supports its logical plausibility.

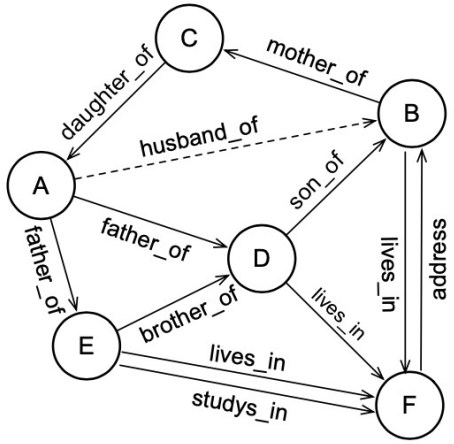
$$\text{score}(u, r_t, v) = \mathbf{W}^T[\mathbf{h}^L_{\mathcal{G}(u,v,r_t)} \oplus \mathbf{h}^L_u \oplus \mathbf{h}^L_v \oplus \mathbf{e}_{r_t}]$$

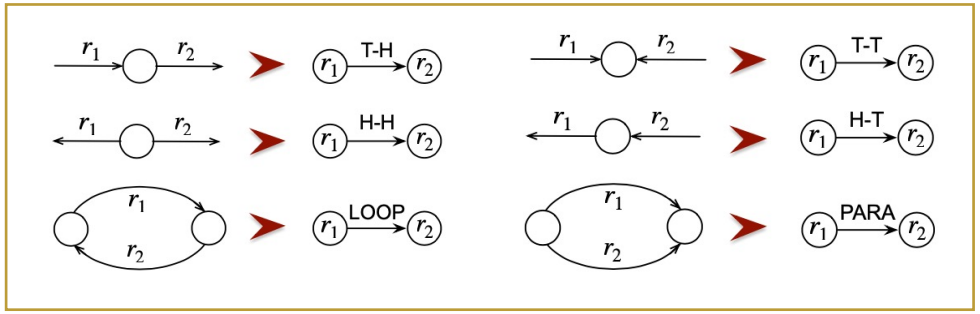
子图表示+头实体表示+尾实体表示+关系表示（随机初始化）

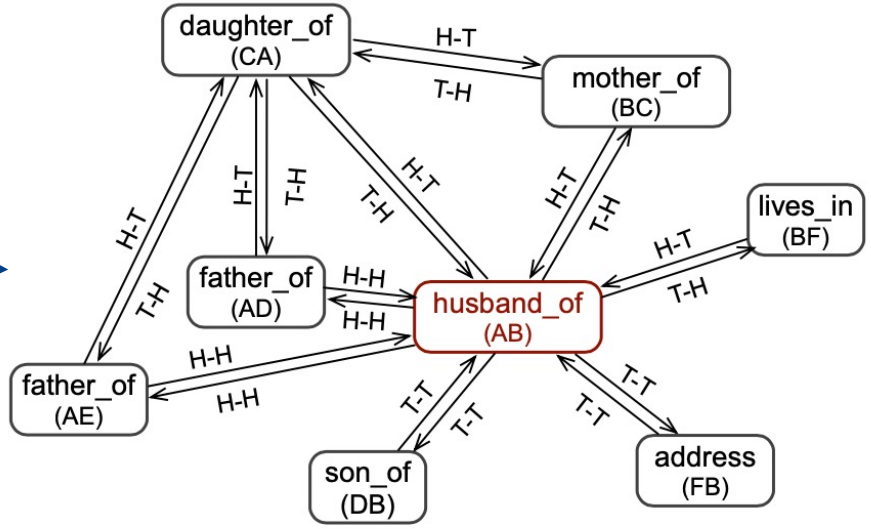
Teru, Komal, Etienne Denis, and Will Hamilton. “**GraIL:** Inductive relation prediction by subgraph reasoning.” ICML 2020.

新实体+新关系：辅助三元组营造推理上下文

- 从三元组周围的局部子图中挖掘推理线索，如可迁移泛化的规则
  - RMPI：直接在关系间进行特征传播，不依赖实体进行推理，泛化至新实体；



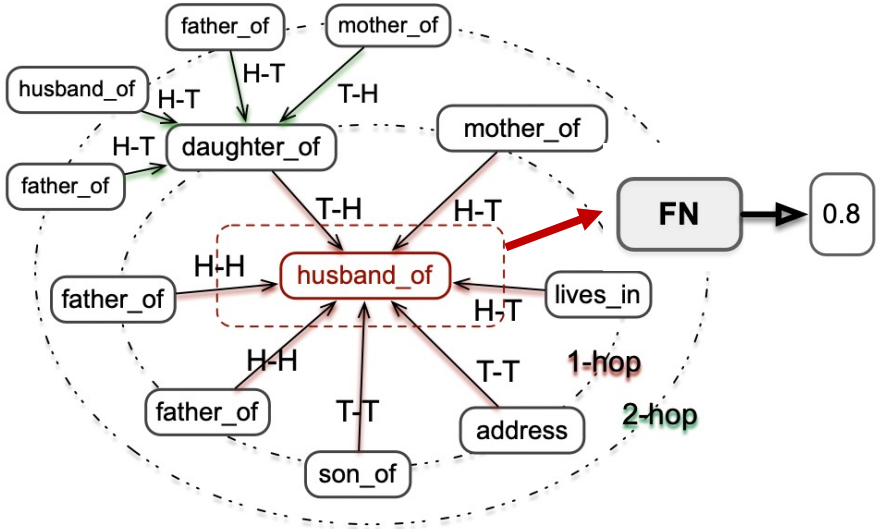




子图转化

关系为节点，关系间关系为边

- 图剪枝：提升计算效率
- 注意力机制：筛选重要邻居

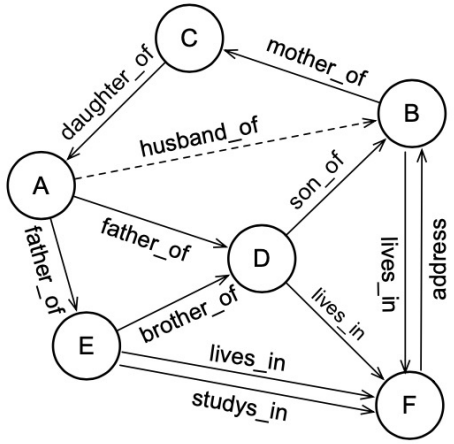


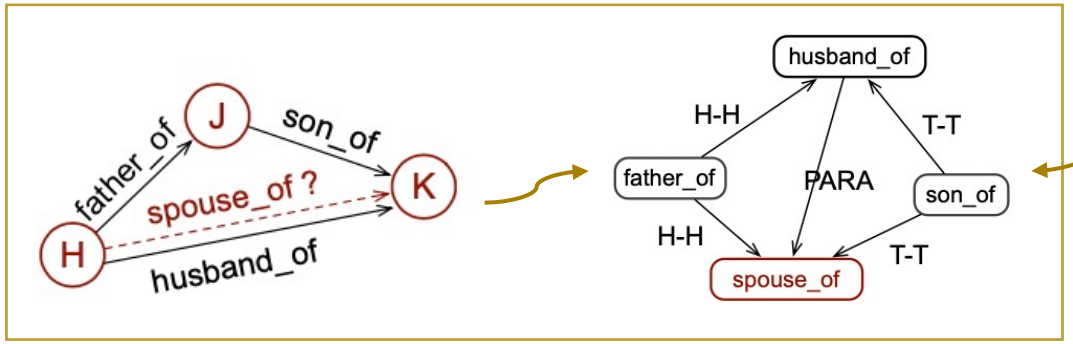
关系导向的图信息传播

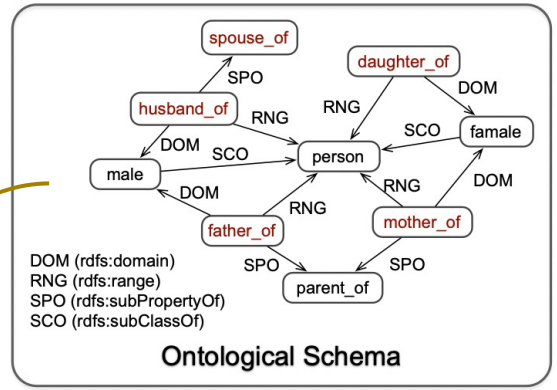
Yuxia Geng, Jiaoyan Chen, Jeff Z. Pan, Mingyang Chen, Song Jiang, Wen Zhang, Huajun Chen. **Relational Message Passing for Fully Inductive Knowledge Graph Completion**. ICDE 2023.

新实体+新关系：辅助三元组营造推理上下文

- 从三元组周围的局部子图中挖掘推理线索，如可迁移泛化的规则
  - RMPI：直接在关系间进行特征传播，可泛化至新关系；

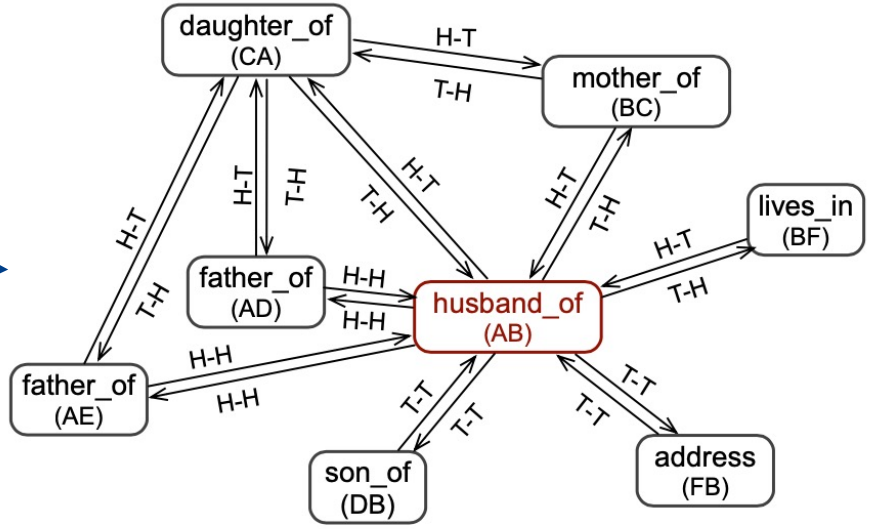


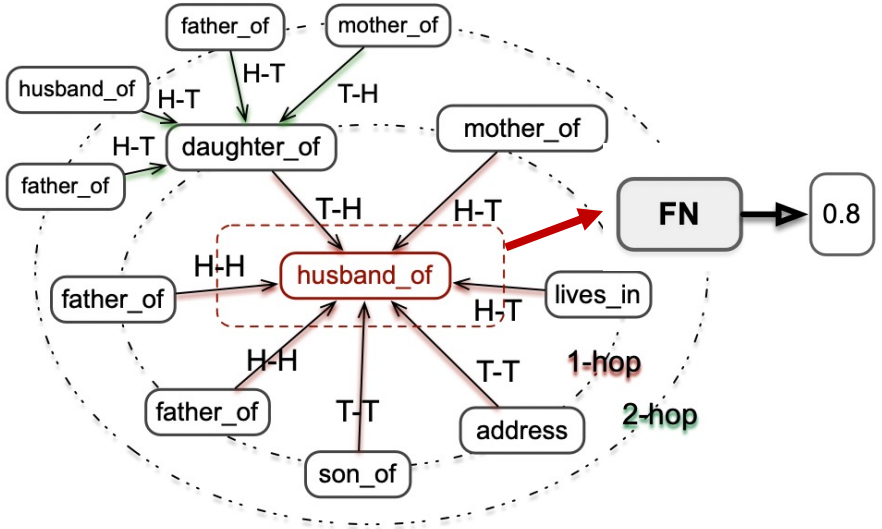




子图转化

关系为节点，关系间关系为边





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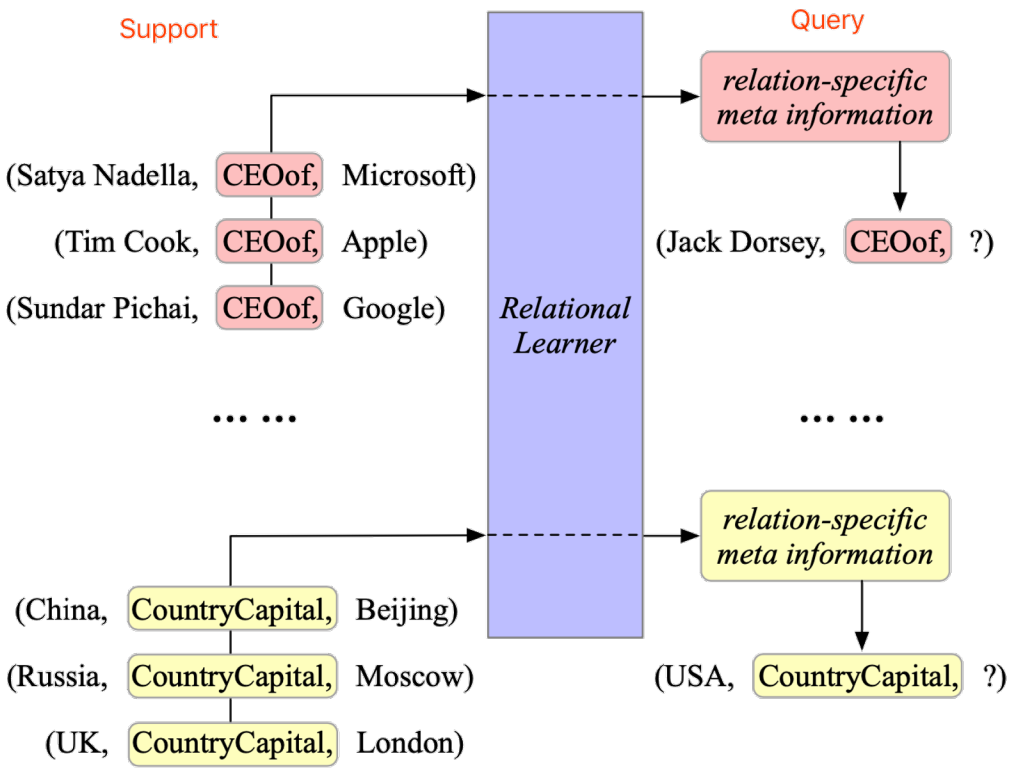
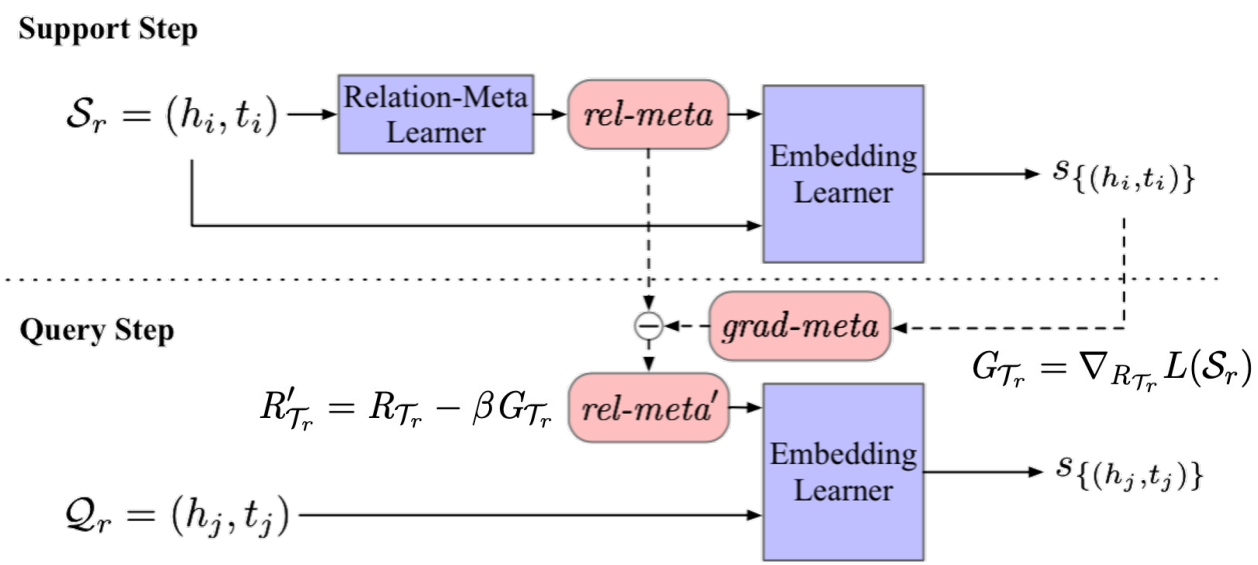
新关系：少量辅助三元组

➢ 元关系学习：在只有少量关系样本（三元组）提供的情况下快速泛化推理三元组的成立概率





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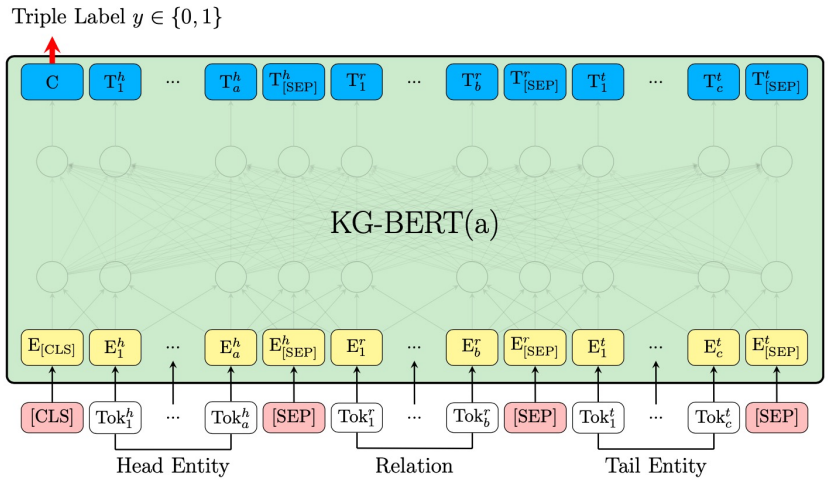
大模型与知识图谱归纳式推理

- **基于外源信息学习新实体/新关系的向量表示**
  - 实体关系的文本、实体的图像
  - 知识图谱本体
  - 额外提供的辅助三元组
    - 辅助三元组，用于建立新旧实体之间的关联，**图神经网络**
    - 辅助三元组，用于建立推理所需的上下文图结构，**图神经网络**
    - 少量辅助三元组，少量推理样本，**元学习**
  - **全归纳式 & 半归纳式**
  - **零样本 & 少样本**

作为大模型下游任务



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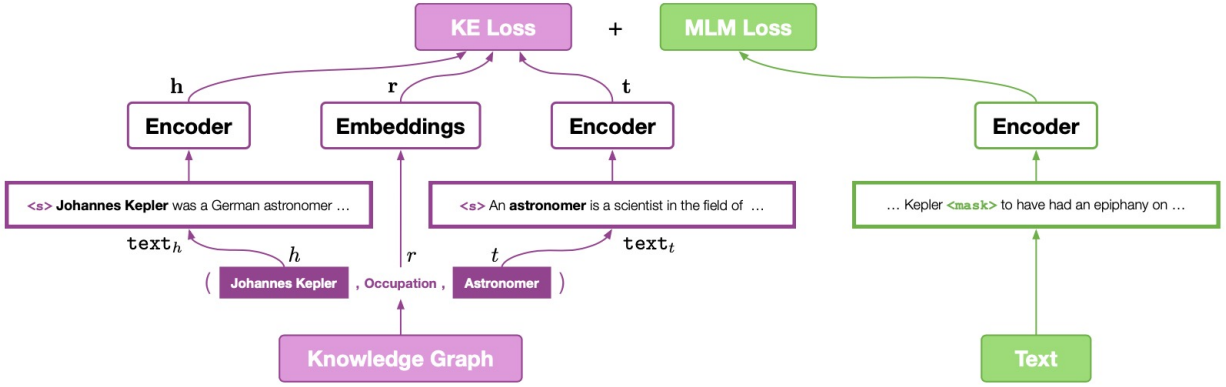

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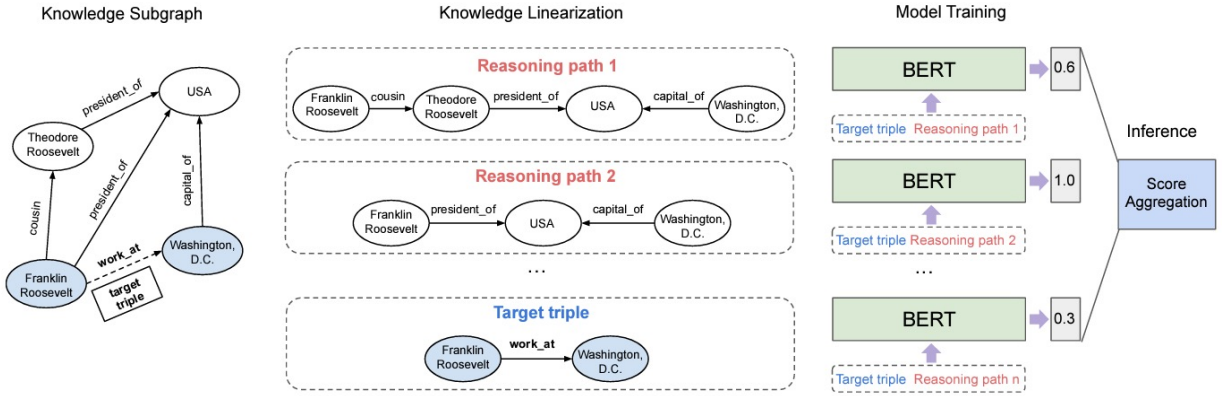

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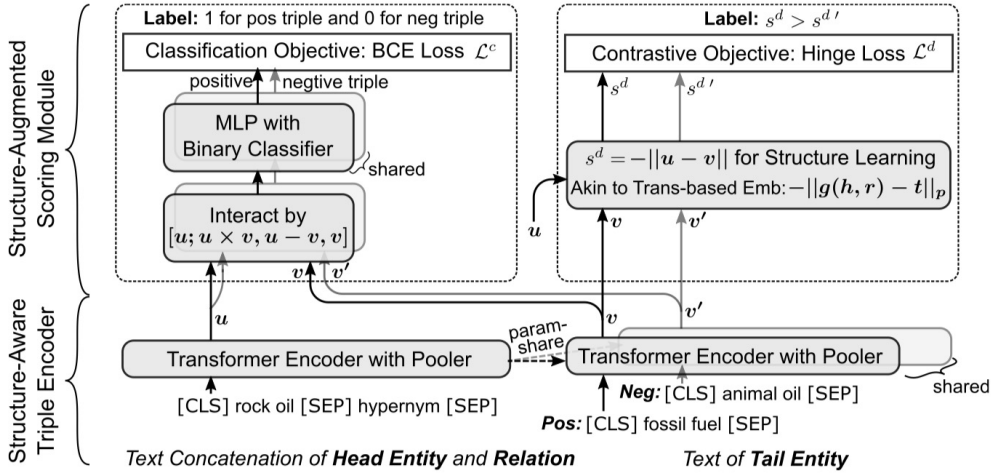


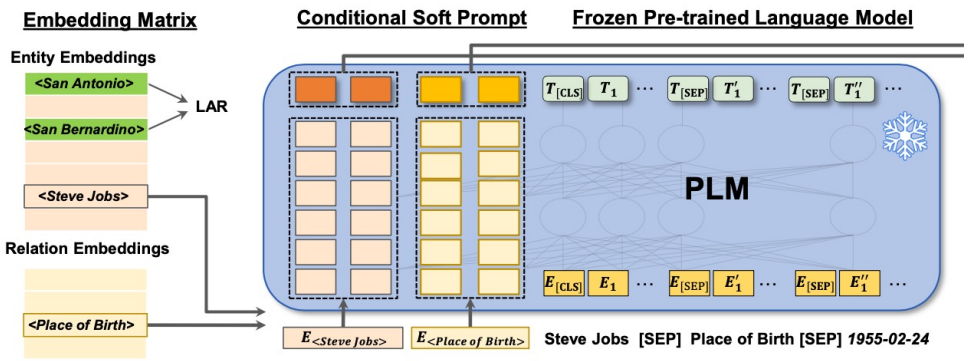
Wang, Bo, et al. "StAR: Structure-augmented text representation learning for efficient knowledge graph completion." WWW 2021.

大模型与知识图谱归纳式推理

- 主要是现有【大模型+直推式推理】方法的延伸
- 主要依赖大模型编码外源文本信息
- 很少利用到辅助三元组中的图结构信息

now we want to know what kind of trophy does entity A win? Given this question, we have the following information as background: A works for entity B, and B often plays against entity C, and C won trophy of superbowl; also, B also known as entity D, and D won trophy of superbowl; and also B won trophy of superbowl. Please answer the question given at the beginning.

Based on the information provided, Entity A works for Entity B, which is also known as Entity D. Both Entity C and Entity D have won the trophy of the Super Bowl. Therefore, it can be inferred that Entity A, being part of Entity B (or D), has also won the trophy of the Super Bowl.



Chen, Chen, et al. “Dipping plms sauce: Bridging structure and text for effective knowledge graph completion via conditional soft prompting.” ACL 2023.

- 基于大模型有效融合归纳推理所需的文本+结构信息？文本编码器 ✗
- 利用大模型本身的知识和推理能力，替代其他（子图）推理模型
- 本体增强的大模型，向大模型引入领域本体知识
- 引入多模态大模型，解决知识图谱归纳式推理问题
- 基于大模型统一不同的归纳式推理范式

THANKS

大模型时代下的知识图谱归纳式推理

Rethinking Inductive KG Reasoning with Language Models

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