# Summary of Knowledge Graph Completion

2024-11-14

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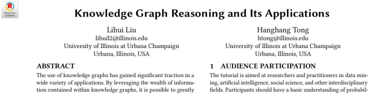
DMAIS

# INDEX

# Introduction

- **Before we start...**
  - □ We'ev been studying about **knowledge graph completion(KGC)** since 2024.07.09.
  - □ We would like to extend our gratitude to the authors and our professor whose materials have made our journey both possible and enriching



Knowledge Graph Reasoning and Its Applications

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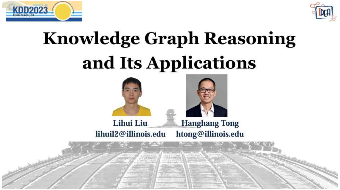
ABSTRACT

The use of knowledge graphs has gained significant traction in a wide variety of applications. By leveraging the wealth of information contained within knowledge graphs, it is possible to greatly

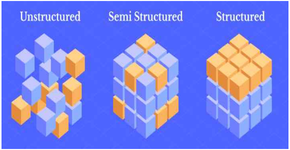
1 AUDIENCE PARTICIPATION

The tutorial is aimed at researchers and practitioners in data mining, artificial intelligence, social science, and other interdisciplinary fields. Participants should have a basic understanding of probabil-

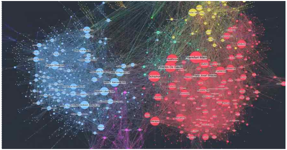


# Introduction

- **What is a KG?**
  - □ First introduced by Google in 2012
  - □ KG, which have long aimed to represent our world through web crawling
  - □ KGs are constructed by using structured, semi structured, unstructured datas



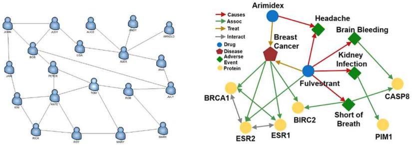

web, JSON, CSV, etc.



NELL, DBpedia, FreeBase, etc.

# Introduction

- **What is a KG?**
  - □ A heterogeneous graph where entities serve as nodes, and edges represent their relationships
  - □ Capable of accommodating **much richer information** than traditional ordinary graphs




△ ordinary graph(left) compared to KG(right)

| Knowledge Graph | Statements | Entities |
|---|---|---|
| YAGO | 120 M | 10 M |
| WIKIDATA | 610 M | 51 M |
| DBpedia | 1.3 B | 6 M |
| GDELT | 3.5 B | 364 M |

△ sizes of popular KGs

# Introduction

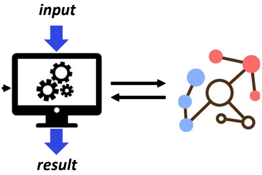
- **Why do we need KGC?**

  □ KGs were mostly incomplete, sparse
  (**60%** of **person** entity did not have **place_of_birth** relation in **DBpedia'14**)

  □ This highlighted the need to fill in gaps to create a more **complete** Knowledge Graph

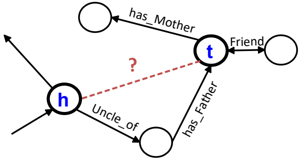
  □ KGC leverages performance in various domains

  ○ information retreival processes in LLMs
  ○ recommender systems
  ○ fact-checking
  ○ question answering

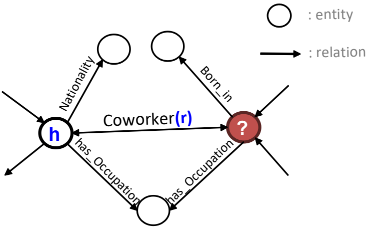


# Introduction

- **Main goal of KGC**
  - □ Given a triplet **(h, r, t)** comprising a head entity **(h)**, a relation **(r)**, and a tail entity **(t)**
  - □ Predict the missing entity or relation to **complete the KG**




△ relation prediction



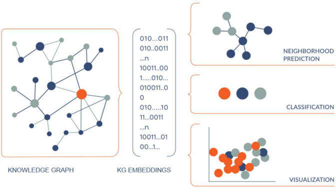

△ link prediction

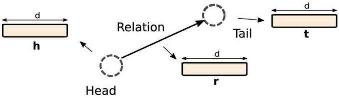
# Introduction

- **General flow of KGC models**
  - □ **Training**
    → Mask the part to be predicted and train the model to rank this masked part as high as possible
  - □ **Testing(**use metrics like AUC, MR, MRR, Hits@k, etc.)
    → Use the trained model to predict the masked part

# Embedding based methods

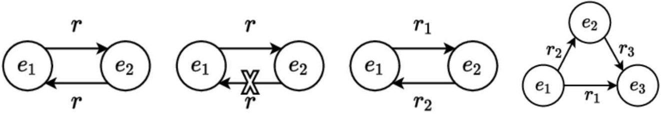
- **What is Embedding based methods?**
  - □ **Goal** : Encode entities and relations as **low-dimensional vectors** in the continuous space
  - □ **Advantages** : Efficient Representation, Ease of representation with vector operation



# Embedding based methods

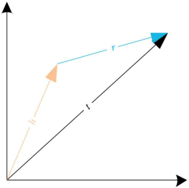
- **Knowledge graph embedding captures KG's patterns**
  - □ Find several relation pattern by embedding entities and relations
  - □ **Symmetry, Antisymmetry, Inversion, Composition** can be captured

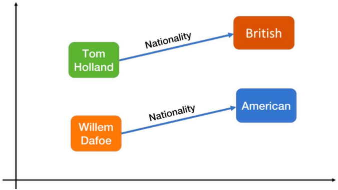



(a) Symmetry (b) Antisymmetry (c) Inversion (d) Composition

# Embedding based methods

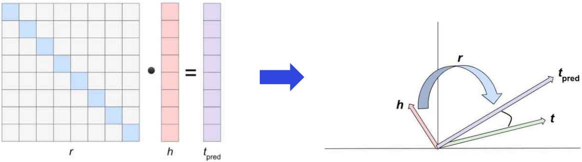
- **TransE (NeurIPS ’13)**
  - □ Make representation with simple operation (light, fast)
  - □ Relation $r$ as a translation from the head entity $h$ to the tail entity $t$ $(t_{pred} = h + r)$



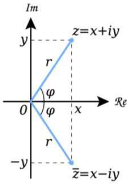
# Embedding based methods

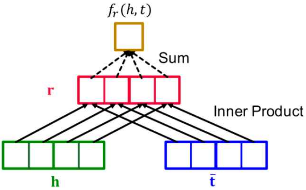
- **DistMult (ICLR '15)**
  - □ Make representation with **dot product**
  - □ Relation $r$ defined as the elementwise weights of the head entity ($h \cdot r = [h_1 \cdot r_1 + \ ... + h_n \cdot r_n]$)



# Embedding based methods

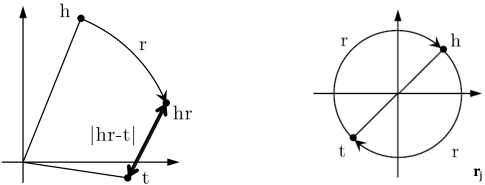
- **ComplEx (ICML '16)**
  - □ Make representation with **Hermitian dot product**
  - □ Using the asymmetry of the Hermitian dot product to represent antisymmetry



# Embedding based methods

- **RotatE (ICLR '19)**
  - ◻ Make representation with **Hadamard product**
  - ◻ Relations modelled as element-wise rotations in complex space ($t_j = h_j r_j, |r_j| = 1$)




$\mathbf{r}_{\mathrm{j}} = -1$ or $\theta_{r,j} = \pi$

# Embedding based methods

- **The patterns a model can capture depends on the representation method**

| Model | Score Function | Symmetry | Antisymmetry | Inversion | Composition |
|---|---|---|---|---|---|
| TransE [2] | $-\|\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|\|$ | ✗ | ✓ | ✓ | ✓ |
| DistMult [3] | $<\mathbf{h},\mathbf{r},\mathbf{t}>$ | ✓ | ✗ | ✗ | ✗ |
| ComplEx [4] | $\mathbf{Re}(<\mathbf{h},\mathbf{r},\bar{\mathbf{t}}>)$ | ✓ | ✓ | ✓ | ✗ |
| RotatE [8] | $-\|\|\mathbf{h}\circ\mathbf{r}-\mathbf{t}\|\|$ | ✓ | ✓ | ✓ | ✓ |

# Embedding based methods(overview)

| TransE | DistMult | ComplEx | RotatE |
|---|---|---|---|
| 2013 | 2015 | 2016 | 2019 |

## ▪ Advantages of KGE

☐ Complex structures can be represented by vector operation

☐ Pattern Learning

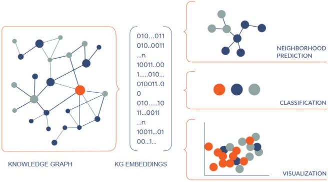
☐ Effect representation

## ▪ Potential bottleneck in KGE

☐ Entity-specific work

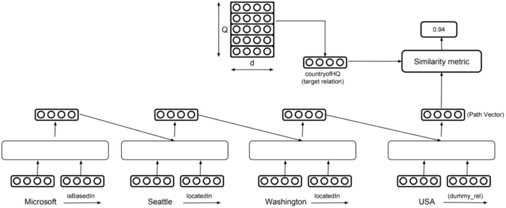
☐ Not applicable in inductive setting

☐ No structural information used



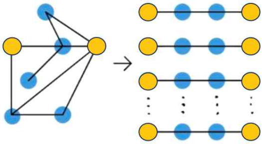
# Path based methods

- **What is Path based methods?**
  - ☐ **Goal** : reach a target entity and inferring new relationships by **exploring multiple paths** in the KG
  - ☐ **Advantages** : inferring without explicit rules



# Path based methods

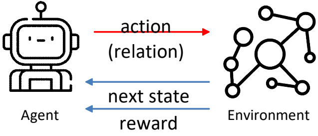
- **PRA (ACL ’11)**
  - ☐ Deriving multiple possible paths between entity pairs through **random walks**
  - ☐ Use supervised training to rank different paths

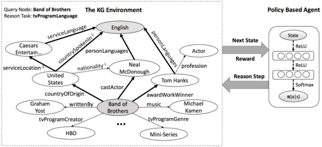


| | Path 1 | Path 2 | ... | Path n | Label |
|---|---|---|---|---|---|
| Query 1 | Score 1.1 | Score 1.2 | ... | Score 1.n | y1 |
| Query 2 | ... | ... | ... | ... | y2 |
| ... | ... | ... | ... | ... | ... |
| Query k | Score k.1 | Score k.2 | ... | Score k.n | yk |

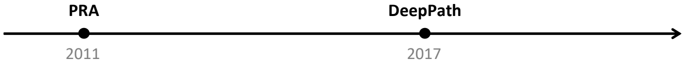
# Path based methods

- **DeepPath (ACL '17)**
  - ☐ Exploring path in KG using **reinforcement learning agent**, modeled as a Markov Decision Process
  - ☐ Agent learns optimal paths to target entities by following reward to discovering efficient paths
  - ☐ Learned paths can be represented as logical rules and used for inferring

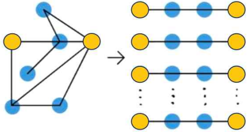


# Path based methods(overview)




- **Advantages of Path based methods**
  - ☐ Generalization and inference with indirect connection between entities
  - ☐ Path can be interpreted as logical rule



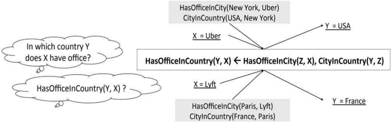
- **Potential bottleneck in Path based**
  - ☐ Only rely on observed paths
  - ☐ Scarcely utilize graph structural informations

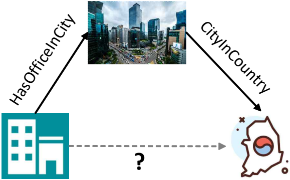
# Rule mining methods

## ▪ What is rule mining?

☐ **Goal** : Aiming to extract **meaningful first order rules** that can be applied to new, unseen data

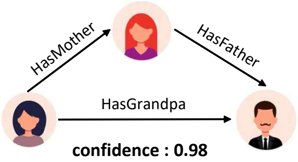
☐ **Advantages** : Generalizable, explainable

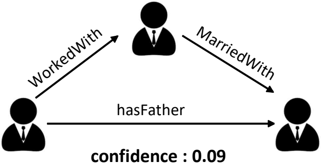


# Rule mining methods

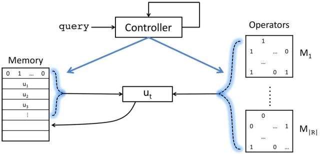
- **Rule mining extracts two components for reasoning**
  - ☐ **The rule itself**(HasOfficeInCountry(Y, X) ⇐ HasOfficeInCity(Z, X), CityInCountry(Y, Z))
  - ☐ **Confidence of individual rule**(how much can we trust it?)



# Rule mining methods

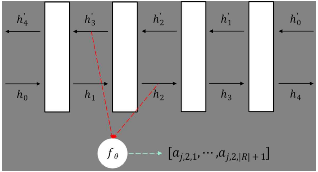
- **NeuralLP(NeurIPS '17)**
  - ☐ **First end-to-end differentiable approach** to learning logical rules
  - ☐ A **LSTM** system that mine rules with varying lengths




$$
\begin{aligned}
\mathbf{h_t} &= \text{update}\left(\mathbf{h_{t-1}}, \text{input}\right) \\
\mathbf{a_t} &= \text{softmax}\left(W\mathbf{h_t} + b\right) \\
\mathbf{b_t} &= \text{softmax}\left(\left[\mathbf{h_0}, \ldots, \mathbf{h_{t-1}}\right]^T \mathbf{h_t}\right)
\end{aligned}
$$

# Rule mining methods

- **DRUM(NeurIPS '19)**
  - ☐ Highlights that NeuralLP can mine **incorrect rules with high confidence**
  - ☐ A **bidirectional RNN** system to reduce the bottleneck of NeuralLP

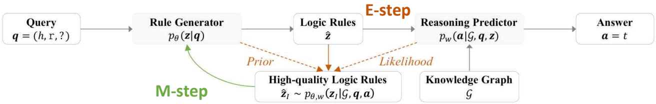



$$\mathbf{h}_i^{(j)}, \mathbf{h}'^{(j)}_{T-i+1} = \mathbf{BiRNN}_j(\mathbf{e}_H, \mathbf{h}_{i-1}^{(j)}, \mathbf{h}'^{(j)}_{T-i}),$$

$$[a_{j,i,1}, \cdots, a_{j,i,|\mathcal{R}|+1}] = f_\theta([\mathbf{h}_i^{(j)}, \mathbf{h}'^{(j)}_{T-i+1}]),$$

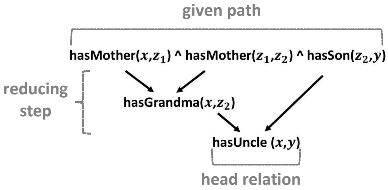
# Rule mining methods

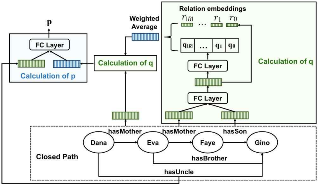
- **RNNLogic(ICLR '21)**
  - ☐ Points out the problem of **large action space** in previous models
  - ☐ An **EM algorithm-based optimization** rule mining model
  - ☐ Seperates rule generating from rule reasoning



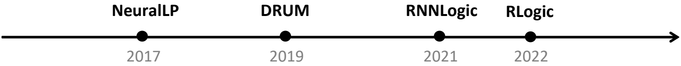
# Rule mining methods

- **RLogic(KDD '22)**
  - ☐ Identifies the issue that **previous models can't mine unseen rules**
  - ☐ Proposes to embrace the deductive reasoning for rule mining
  - ☐ A recursive framework that reduces a path to a single head relation



# Rule mining methods(overview)

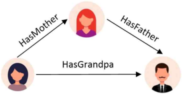



## ▪ Advantages of rule mining

☐ Mined rules can be generalized

☐ Rules are explainable and understandable

☐ Entity inductive framework




**VS**

[0.013472648337483406, -0.005545202642679214, 0.04156069457530975,
-0.01467960886657238, -0.007239829283207655, -0.008201991207897663,
0.009404981508851051, -0.02347548119723797, -0.005465532653033733,
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0.009313264861702919, 0.016721446067094803, -0.04639590531587601, . . . ]

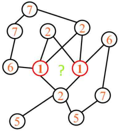
## ▪ Potential bottleneck in rule mining

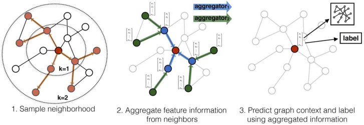
☐ Rules are inherently discrete

☐ The approach does not align well with the incompleteness of KG

# GNN based methods

- **What is GNN based methods?**
  - ☐ **Goal** : Integrates GNN approaches(SEAL, GraphSAGE, etc.) into KGC
  - ☐ **Advantages** : Leverages structural information of graph



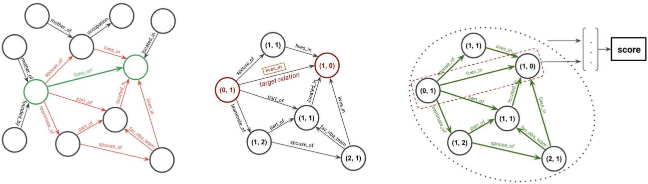




△ structural node labelling(SEAL)

△ aggregating process(GraphSAGE)

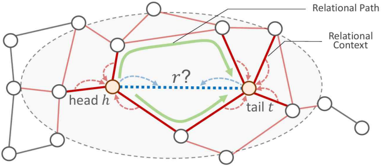
# GNN based methods

- **GraIL(ICML '20)**
  - ☐ Adopts subgraph reasoning around target nodes to enhance relational understanding
  - ☐ Performs GNN message passing with structurally labeled nodes to infer missing relations

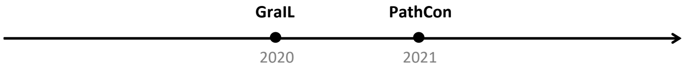


# GNN based methods

- **PathCon(KDD '21)**
  - ☐ Acknowledges that reasoning can be decomposed into **context** and **path**
  - ☐ **Context** : defines the entity type of target nodes through relatoinal message passing
  - ☐ **Path** : defines the reletive position between target nodes



# GNN based methods(overview)

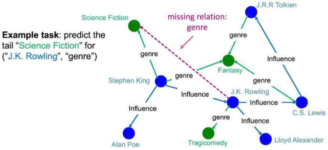


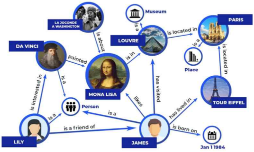

- **Advantages of GNN based methods**
  - ☐ Combines successful methods previously introduced for ordinary graphs
  - ☐ Entity inductive framwork

- **Potential bottleneck in GNN based methods**
  - ☐ Challenging since edge type also needs to be modeled

# Conclusion

**We view** knowledge graph completion not merely as a method for filling gaps in the knowledge graph, but as a tool **enabling AI models to understand** relationships between real-world entities, ultimately fostering a deeper understanding of the world we live in



# Thank You!