INFR11215 Knowledge Graphs

Combined KG Reasoning

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Lecture Outline

• Motivation
• Discussions on Schema-aware KG Embedding
Motivations

• Pros of KG embeddings:
  – Help to address the incompleteness
  – Useful in many downstream applications
    like link prediction, similarity search and
    question answering

• Cons of KG embeddings:
  – typically only consider relation assertions
  – do not consider schema
    • Why is it a problem?
    • If it is a problem, how to address it?

Lecture Outline

• Motivation

• Discussions on Schema-aware KG embedding
Brief Summary of KGE for LP

- Link prediction: can be cast as a learning to rank problem

\[ \phi_{spo} = \phi((s, p, o); \Theta) \]

- KGE for link prediction: 2-layer neural network architecture
  - Encoding layer
  - Scoring layer

\[ \phi((s, p, o); \Theta) = \phi_p(e_s, e_o) \]
\[ e_s, e_o = \psi(s), \psi(o) \]

- Loss function require both positive and negative samples

Why Ignoring Schema is a Problem?

- Closed world assumption
- Limited expressiveness of KGE models
- Inconsistency
Closed World Assumption

- Key question: how to pick samples
  - Positive samples are easy
  - Negative samples are a lot trickier, as all input triples are positive
- Closed World Assumption (CWA) is used to pick negative samples:
  - given a KG G, its schema S and a new triple \((s,p,o)\): if \((s,p,o) \in G\), then \((s,p,o)\) is correct; otherwise, \((s,p,o)\) is incorrect
  - Procedure: given any \((s,p,o)\), replace \(s\) with \(s'\) s.t. \((s',p,o) \notin G\)

Example: Closed World Assumption

**Example 1:** if the KG contains the triple \((John, likes, Ice_Cream)\), under the CWA, the negative sample \((John, likes, Pizza)\) would be unequivocally considered as false, suggesting that John does not like pizza.

**Example 2:** Given a positive triple \((English_Americans, population_place, New_England)\) in DB15K dataset, the CWA negative sampling strategy replaces the tail entity with random entities, such as:
- \((English_Americans, population_place, Hawaii)\)
- \((English_Americans, population_place, Arizona)\)
- \((English_Americans, population_place, New York metropolitan area)\)
- \((English_Americans, population_place, Vietnam)\)
- \((English_Americans, population_place, Uruguay)\)
- \((English_Americans, population_place, Seattle metropolitan area)\)
- \((English_Americans, population_place, Chicago metropolitan area)\)
- \((English_Americans, population_place, Guatemala)\)

However, there are a few false negative triples.
Alternatives to Closed World Assumption

- Schema-aware Closed World Assumption (SCWA): given a KG G, its schema S and a new triple (s,p,o): if (s,p,o) ∈ Closure(G U S), then (s,p,o) is correct; otherwise, (s,p,o) is incorrect (Wang et al. 2023)

- Open World Assumption: given a KG G, its schema S and a new triple (s,p,o): if S U G U (s,p,o) ꞁ ≠ ꞁ, then (s,p,o) is correct; otherwise, (s,p,o) is incorrect

Limited expressiveness

- Fully expressiveness not enough
  - Given T* positive and T- negative sample sets
  - ∀(s,p,o) ∈ T*, Φ_p(e_s, e_o) ≤ λ_p
  - ∀(s,p,o) ∈ T-, Φ_p(e_s, e_o) > λ_p

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From Sun et al. - RotatE: Knowledge Graph Embeddings by Relational Rotation in Complex Space
Inconsistency

Exploration for dbo:locationRange dbo:organization
1) dbo:Broadcaster DisjointWith dbo:location
   In NO other justifications
2) dbpedia:Lower_Hutt dbo:broadcastArea dbpedia:Wellington
   In NO other justifications
3) dbo:broadcastArea Domain dbo:Broadcaster
   In NO other justifications
4) dbpedia:Lower_Hutt Type dbo:location
   In NO other justifications

Note: the two relation assertions have been removed in latest DBpedia release, but still exist in DB15K dataset.

How to Address the Expressiveness Issue

- Incorporate schema information in loss function good approaches expected to be applicable to different KGE methods

- Combine symbolic reasoning with KGE Use OWA to check if the triples learned from KGE methods are consistent with the schema
  - Bonus: consistent triples can be combined with existing triples and schema to infer further triples
Incorporate Schema Information in Loss Function

- Example schema axioms:
  - Relation equivalence: \( p \equiv q \) (\( p \sqsubseteq q, q \sqsubseteq p \))
    \[
    \phi((s, p, o); \Theta) = \phi((s, q, o); \Theta) \quad \forall s, o \in \mathcal{E}.
    \]
  - Inverse relations: \( p \equiv q' \) (\( p \sqsubseteq q', q' \sqsubseteq p \))
    \[
    \phi((s, p, o); \Theta) = \phi((o, q, s); \Theta) \quad \forall s, o \in \mathcal{E}.
    \]
- Scalable implementation of such revised scoring functions often demands KGE dependent revisions
- Optional reading:
  [https://link.springer.com/chapter/10.1007/978-3-319-71249-9_40](https://link.springer.com/chapter/10.1007/978-3-319-71249-9_40)

Combine Symbolic Reasoning with KGE

- KGE training with ACC for sampling
- Predict
- Expanded KG
- ACC
- Updated KGE

- Output KG
- Schema-correct triples
- Schema-inconsistent triples (Neg candidates for next round training)
- Schema-correct triples (Pos)
- Schema-inconsistent triples (Neg)

ACC: Approximated Consistency Checking

Optional reading: [https://knowledge-representation.org/z.z.pan/pub/SICKLE2023.pdf](https://knowledge-representation.org/z.z.pan/pub/SICKLE2023.pdf)

- Schema-correct: consistent with the schema of the Knowledge Graph and satisfying the constraints, such as domain and range.
- Schema-unknown: they are consistent with the schema, but not yet satisfying the constraints, due to lack of some type information for their heads or tails, i.e., neither schema-correct nor schema-incorrect.
- Schema-inconsistent: not consistent with the schema.
Lecture Outline

- Motivation: KGE lack significant expressiveness
- Introduction: Limitations of classic KGE methods
- Focus: Solutions of these limitations
- Practical
  - Combine symbolic reasoning with KGE
  - Schema aware zero shot learning
- Next time we introduce tractable Description Logic EL