



Knowledge Graph Embedding via Metagraph Learning

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Knowledge Graphs



• Human knowledge as a directed graph

• Each fact is represented as a triplet (head entity, relation, tail entity)



(Joe Biden, is Politician of, USA)
(USA, is Located in, America)
(Canada, is Located in, America)
(USA, shares Border with, Canada)
(Olympic Games, was Held in, USA)
(Olympic Games, was Held in, Canada)

Knowledge Graph Embedding

• Representation Learning Technique

- Projects entities and relations into a continuous feature space.
- Applicable to solving diverse problems such as link prediction.

• Knowledge Graph Embedding Methods

- Translational Distance Models (e.g., TransE, TransH, TransR)
- Semantic Matching Models (e.g., DistMult, RotatE)





Entity and relation space

Intuition

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• Semantic closeness can be inferred by the structural similarity between entities.

 If two entities share the same tail entity or the same head entity with the same relation, they might belong to the same semantic category.



'USA' and 'Canada' are structurally similar.

- They share the same tail entity 'America' with the relation 'is Located in'.
- They share the same head entity 'Olympic Games' with the relation 'was Held in'.

Overview

Hypergraph representation of a knowledge graph

- Connect a set of semantically close entities by looking at the structure of a knowledge graph.
- o Group similar entities by hypergraph clustering.
 - Based on the newly defined affinity metric, perform hypergraph clustering.



Overview

o Metagraph embedding

- Form super-entities by merging entities in the same group and learn embeddings.
- Pre-train a knowledge graph embedding model
 - Initialize corresponding entities and relations with the learned representations.



Hypergraph Representation

• Connect a set of entities that share the same head (tail) entity with the same relation.

- A hyperedge can connect an arbitrary number of nodes.
- Define a new affinity score between two entities \rightarrow reflects the structural similarity
 - Affinity between entities $i \& j: a_{ij} = \sum_{l \in \mathcal{L}} 1/d_l^2$ where \mathcal{L} is the set of hyperedges that contain both i and j, and d_l indicates the number of entities included in the hyperedge l.



Grouping Entities

Perform hypergraph clustering with the normalized affinity scores to group entities.

Normalize the affinity scores with respect to individual entities.

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Metagraph of a Knowledge Graph

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- Merge entities in the same group to form a super-entity.
- Metagraph \rightarrow preserves a core structure of the given knowledge graph.
 - Within-group triplets are dropped.
 - Between-group triplets are probabilistically dropped.



Pre-training of Knowledge Graph Embedding

- Run a knowledge graph embedding method on the metagraph.
- Initialize the corresponding entities and relations in the original knowledge graph with the learned representations on the metagraph.
 - Entities in the same super-entity are initialized with the same representations.



Top Similar Entities from NELL-995



o Target entity: emotion_thankfulness

- emotion_graditude, emotion_admiration, emotion_happiness, emotion_joy, emotion_deep_love, emotion_jealousy, emotion_thanks
- O Target entity: software_microsoft_word
 - software_internet_explorer, software_microsoft_frontpage, software_microsoft_powerpoint, software_notepad, software_autocad
- **o** Target entity: sport_american_football
 - sport_ski, sport_scout, sport_skiing, sport_golf, sport_judo

Datasets

- We cluster the entities so that the size of the metagraph becomes about half of the original knowledge graph in terms of the number of triplets in the train set.
 - We perform clustering only using the train set.

| | | Train set | | | Validation set | | | Test set | | |
|----------|-------------|-----------|-------|---------|----------------|-----|--------|-----------------|-----|--------|
| | | V | R | E | V | R | E | V | R | E |
| FB15K | Original KG | 14,951 | 1,345 | 483,142 | 13,292 | 916 | 50,000 | 13 <i>,</i> 584 | 961 | 59,071 |
| | Metagraph | 10,387 | 1,142 | 224,824 | 8,377 | 686 | 21,778 | 8,611 | 703 | 25,433 |
| NELL-995 | Original KG | 74,432 | 200 | 149,678 | 765 | 12 | 543 | 3,747 | 12 | 3,992 |
| | Metagraph | 48,693 | 200 | 67,588 | 382 | 12 | 261 | 2,387 | 12 | 2,118 |
| WN18 | Original KG | 40,943 | 18 | 141,442 | 7,802 | 18 | 7,802 | 7 <i>,</i> 845 | 18 | 5,000 |
| | Metagraph | 27,250 | 18 | 63,423 | 3,695 | 18 | 3,695 | 3,689 | 18 | 2,227 |

Experimental Results



o Link Prediction Results

• A positive gain indicates that our method is better than the original model.

| | | MR (↓) | MRR (†) | Hit@10 (†) | Total Gain (\uparrow) |
|-------|-------------------|--------|------------------|---------------|---------------------------|
| | TransE | 89.0 | 0.596 | 0.733 | |
| | meta-TransE | 75.0 | 0.551 | 0.798 | |
| | Gain (†) | 15.8% | -7.5% | 8.8% | 17.1% |
| | DistMult | 106.4 | 0.414 | 0.644 | |
| FB15K | meta-DistMult | 143.7 | 0.541 | 0.786 | |
| | Gain (†) | -35.0% | 30.8% | 21.9 % | 17.7% |
| | RotatE | 34.4 | 0.691 | 0.869 | |
| | meta-RotatE | 33.6 | 0.690 | 0.871 | |
| | Gain (†) | 2.1% | -0.1% | 0.2% | 2.2% |

Experimental Results

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• Link Prediction Results

• A positive gain indicates that our method is better than the original model.

| | | MR (↓) | MRR (\uparrow) | Hit@10 (†) | Total Gain (\uparrow) |
|----------|---------------|---------|--------------------|--------------|---------------------------|
| | TransE | 7202.4 | 0.278 | 0.477 | |
| | meta-TransE | 6507.5 | 0.287 | 0.434 | |
| | Gain (†) | 9.6% | 3.3% | -9.1% | 3.8% |
| | DistMult | 10312.7 | 0.298 | 0.388 | |
| NELL-995 | meta-DistMult | 8046.0 | 0.288 | 0.397 | |
| | Gain (†) | 22.0% | -3.6% | 2.3% | 20.7% |
| | RotatE | 9243.9 | 0.350 | 0.428 | |
| | meta-RotatE | 8618.7 | 0.352 | 0.435 | |
| | Gain (†) | 6.8% | 0.7% | 1.8% | 9.3% |

Experimental Results



o Link Prediction Results

• A positive gain indicates that our method is better than the original model.

| | | MR (↓) | MRR (†) | Hit@10 (†) | Total Gain (†) |
|------|-------------------|--------|------------------|--------------|------------------|
| | TransE | 210.4 | 0.521 | 0.943 | |
| | meta-TransE | 185.9 | 0.535 | 0.949 | |
| | Gain (†) | 11.6% | 2.7% | 0.7% | 15.0% |
| | DistMult | 301.1 | 0.320 | 0.550 | |
| WN18 | meta-DistMult | 289.1 | 0.463 | 0.732 | |
| | Gain (†) | 4.0% | 44.7% | 33.2% | 81.9% |
| | RotatE | 76.681 | 0.661 | 0.882 | |
| | meta-RotatE | 73.718 | 0.655 | 0.884 | |
| | Gain (†) | 3.9% | -0.9% | 0.2% | 3.2% |

Summary



- By identifying a set of structurally similar entities, group semantically close entities.
- Construct the metagraph of a knowledge graph \rightarrow a pre-training method
- Empirically, our pre-training method improves the link prediction performance.
- Future work: overlapping clustering and multi-level clustering



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