EmbedS: Scalable and Semantic-Aware Knowledge Graph Embeddings

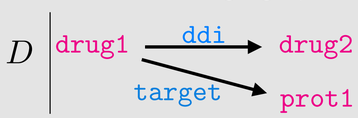
Gonzalo I. Diaz[1], Achille Fokoue[2], Mohammad Sadoghi[3]

1 University of Oxford 2 IBM T.J. Watson Research Center

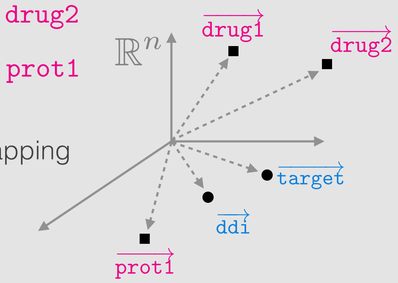
3 University of California, Davis

Knowledge Graphs and Translational Embeddings

Assume a knowledge graph:



And an embedding mapping **entities** and **relations**:

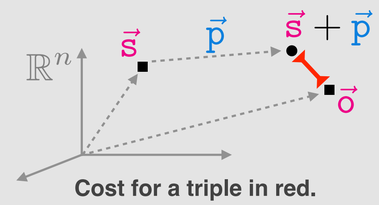


These models represent **relations** as a translational vector. Learning is achieved by minimizing the cost:

$$\mathcal{L} = \sum_{(s,p,o)} \left[||(\vec{s}+\vec{p}) - \vec{o}|| - ||(\vec{s}'+\vec{p}) - \vec{o}'|| + \gamma \right]_+$$

This model, **TransE** [1], was inspired by word2vec. The cost per triple is:

$$\mathcal{L}_{(s,p,o)} = ||(\vec{s}+\vec{p}) - \vec{o}||$$



Cost for a triple in red.

1

Ontology-aware embeddings

Ontology-unaware embeddings may violate semantics:

Ontology-aware	Ontology-unaware
(drug1, target, prot1)	(uri1, uri2, uri3)
(prot1, rdf:type, Prot)	(uri3, uri4, uri5)
(target, rdfs:range, Prot)	(uri2, uri6, uri5)

This can result in inferred triples (i.e. facts) that violate the semantic constraints of the graph:

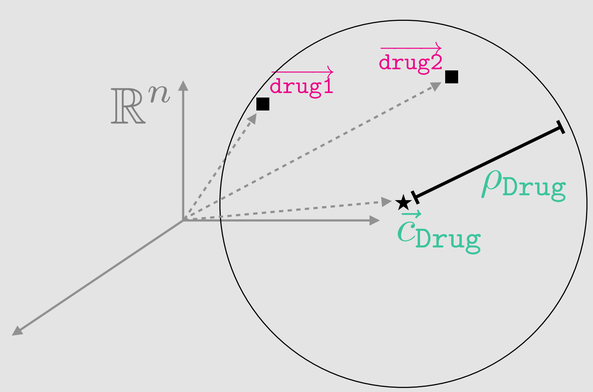
(uri7, uri2, uri1) → (drug2, target, drug1)

violates semantics!

2

EmbedS modeling

In EmbedS, we model **entities** as points, **classes** as sets of points (an *n*-sphere, with a central vector and a radius), and **properties** as sets of pairs of points (modeled analogously).



3

EmbedS Cost Model and Performance

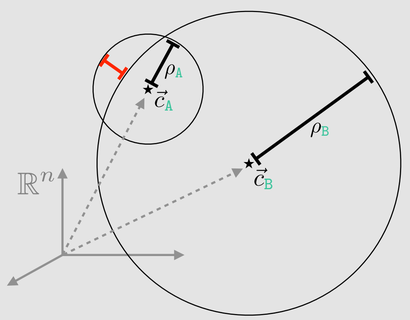
EmbedS assigns a cost for violating semantic constraints. For example:

Example: for an RDFS triple

(A, rdfs:subClassOf, B)

the cost assigned is shown as a red error bar.

4



Hyper-parameter optimization: Random search [2].

Scalability: EmbedS uses Approximate Nearest Neighbor indexing for scalable learning.

Performance: Initial experimental evaluation on a benchmark dataset and an ad hoc dataset show competitive performance.

wn18 dataset:
hits@10: 94.9%, MRR: 0.560 (HMR: 1.79)

P = 84.2% and a Recall = 83.9%, f-measure: 84.0% (optimizing the geometrical interpretation)

dbpedia_v2 dataset:
EmbedS: hits@10: 22.7%, MRR: 0.133 (HMR: 7.52)

References:

[1] A. Bordes, N. Usunier, A. García-Durán, J. Weston, and O. Yakhnenko. Translating Embeddings for Modeling Multi-relational Data. In NIPS'13.

[2] J. Bergstra and Y. Bengio. Random Search for Hyper-Parameter Optimization. JMLR'12.