Relation Prediction as an Auxiliary Training Objective for Improving Multi-Relational Graph Representations

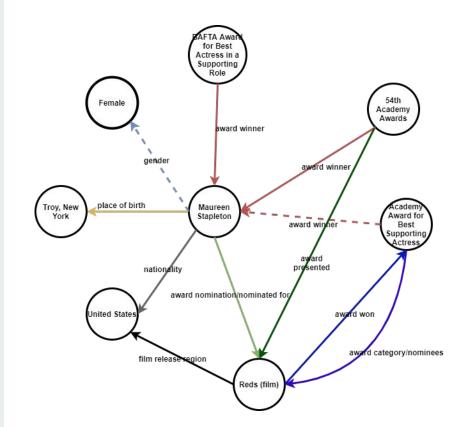
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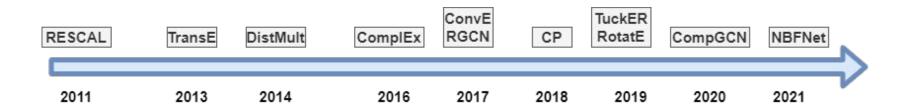
Knowledge Base Completion (KBC)

The task of KBC demands good representation learning on multi-relational graphs.

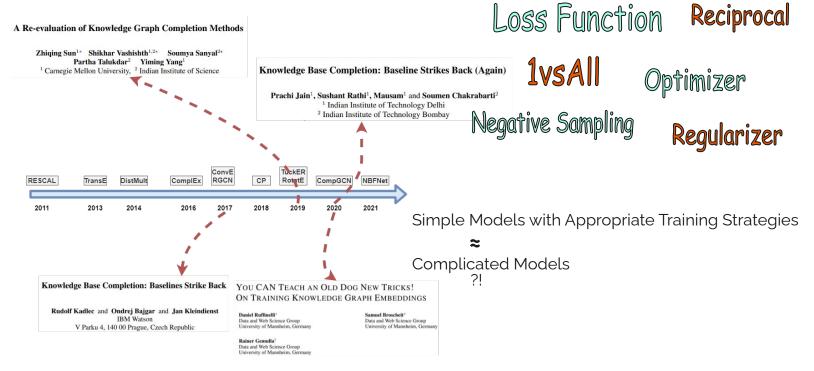


History of KBC Models

Models get more and more complex ...



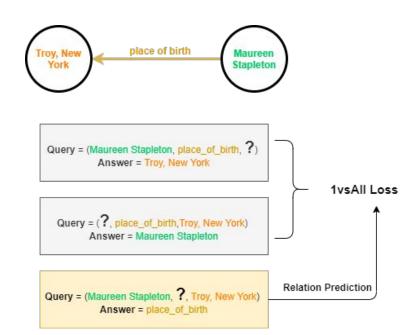
Re-evaluation of KBC Models



Relation Prediction as An Auxiliary Training Objective for KBC

A new self-supervised training objective

- not only predicting entities
- but also predicting relations



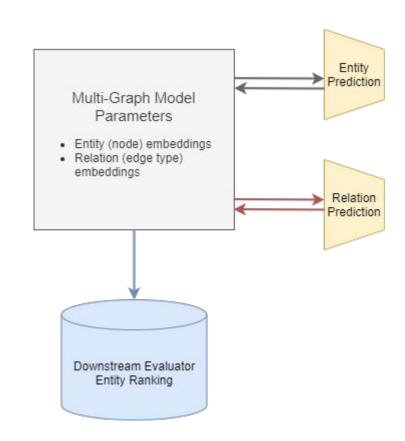
Including Relation Prediction into 1vsAll Objective

$$\arg \max_{\theta \in \Theta} \sum_{\langle s, p, o \rangle \in \mathcal{G}} [\log P_{\theta}(s \mid p, o) + \log P_{\theta}(o \mid s, p) + \lambda \log P_{\theta}(p \mid s, o)]$$
with
$$\log P_{\theta}(p \mid s, o) = \phi_{\theta}(s, p, o) - \log \sum_{p' \in \mathcal{R}} \exp \left[\phi_{\theta}(s, p', o)\right],$$

λ: hyper-parameter balancing the entity prediction and relation prediction

Experiments

How does relation prediction impact various models on different datasets?



Experimental Setup

Models RESCAL, Complex, CP, TuckER

extensive hyper-parameters search based on validation set ≈ 41,316 runs

Dataset	$ \mathcal{E} $	$ \mathcal{R} $	#Train	#Validation	#Test	
Nations	14	55	1,592	100	301	
UMLS	135	46	5,216	652	661	
Kinship	104	25	8,544	1,068	1,074	
WN18RR	40,943	11	86,835	3,034	3,134	
FB15k-237	27,395	237	272,115	17,535	20,466	
Aristo-v4	44,950	1,605	242,594	20,000	20,000	

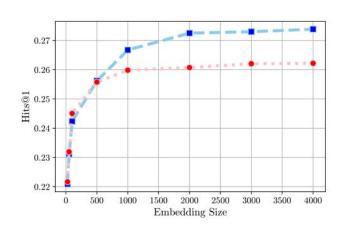
Test Performance on All Datasets

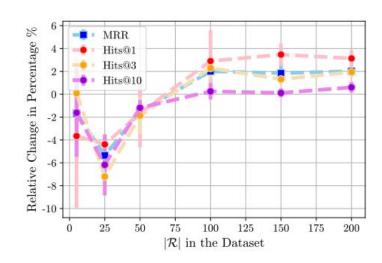
Dataset	Entity Prediction	Relation Prediction	MRR	Hits@1	Hits@3	Hits@10	Dataset	Entity Prediction	Relation Prediction	MRR	Hits@1	Hits@3	Hits@10
Kinship	×	✓	0.920	0.867	0.970	0.990	WN18RR	X	✓	0.258	0.212	0.290	0.339
Manhala E	V	×	0.897	0.835	0.955	0.987		✓	×	0.487	0.441	0.501	0.580
	✓	✓	0.916	0.866	0.964	0.988		V	✓	0.488	0.443	0.505	0.578
Nations	×	✓	0.686	0.493	0.871	0.998	FB15K-237	×	✓	0.263	0.187	0.287	0.411
	✓	×	0.813	0.701	0.915	1.000		V	×	0.366	0.271	0.401	0.557
	✓	✓	0.827	0.726	0.915	0.998		V	✓	0.388	0.298	0.425	0.568
UMLS	×	V	0.863	0.795	0.914	0.979	Aristo-v4	×	✓	0.169	0.120	0.177	0.267
	V	×	0.960	0.930	0.991	0.998		✓	×	0.301	0.232	0.324	0.438
	V	✓	0.971	0.954	0.986	0.997		V	✓	0.311	0.240	0.336	0.447

Test Performance Across Various Models, λ=1

Model	Relation Prediction	MRR	Hits@1	Hits@3	Hits@10
CD	×	0.356	0.262	0.392	0.546
CP	✓	0.366	0.274	0.401	0.550
G 15	×	0.366	0.271	0.401	0.557
ComplEx	✓	0.382	0.289		0.568
PEGGIA	×	0.356	0.266	0.390	0.532
RESCAL	✓	0.359	0.271	0.395	0.533
72 1,112	×	0.351	0.260	0.386	0.532
TuckER	V	0.354	0.264	0.395	0.535

Ablation Study: Embedding Size & Number of Relation Types





Summary

Relation Prediction as an Auxiliary Objective for Training KBC Models

Conclusion

- a new self-supervised objective for training KBC models
- up to 9.9% boost in Hits@1 on FB15k-237

Future Work

- extend to more complex models
- downstream applications besides link prediction
 - o node classification

Thank you:)

Q&A