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Knowledge Graph Completion

■ Evaluation Procedure

■ Filtered Setting

Breaking Ties

■ The Open World

KNOWLEDGE GRAPH COMPLETION

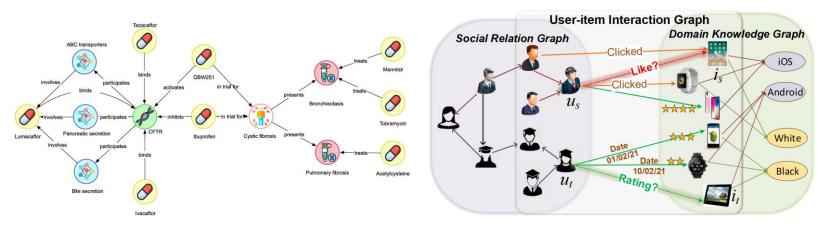


What is a Knowledge Graph(KG)?

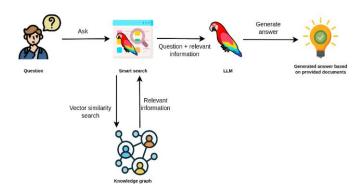
- ☐ Heterogeneous graph consisting of **entities**(nodes) and **relations**(edges)
- ☐ **Triple** = (head entity, relation, tail entity)

<Drug Discovery>

 \square Rich representation \rightarrow applied in various domains







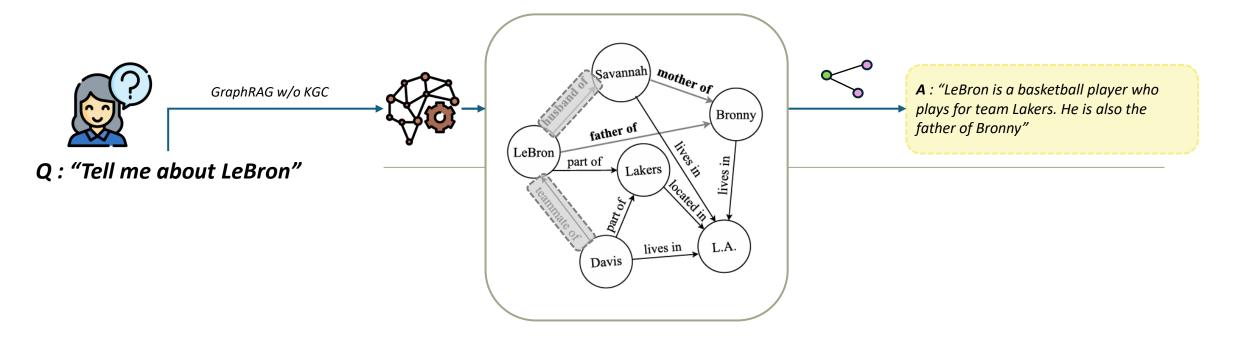
<GraphRAG>

KNOWLEDGE GRAPH COMPLETION



Missing Facts in KGs

- ☐ In Freebase and DBpedia, more than 66% of the person entities are missing a birthplace
- ☐ Greatly hinder the performance of systems that rely upon it



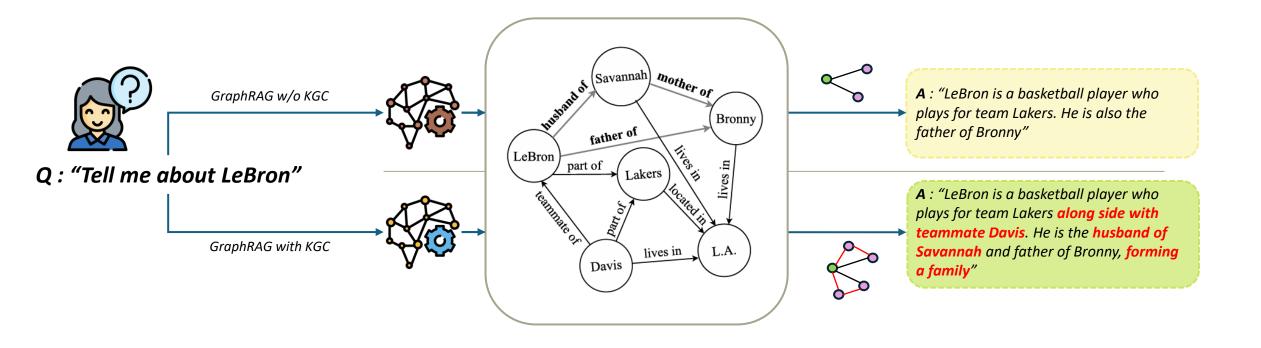
KNOWLEDGE GRAPH COMPLETION



Knowledge Graph Completion(KGC)

- ☐ KGC model to automatically fill missing links has been extensively studied
- □ Normally two tasks exist, link prediction(entity prediction) and relation prediction

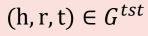
link prediction : (h, r, ?) or (?, r, t) \rightarrow predict "?"



EVALUATION PROCEDURE



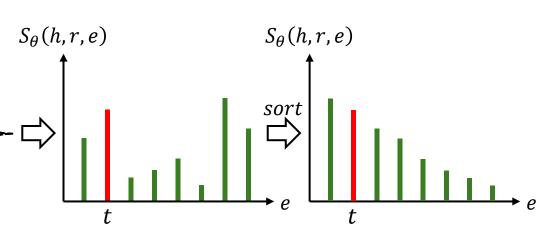
Evaluation Procedure of KGC Models



 $S_{\theta}: (h, r, t) \rightarrow score \in \mathbb{R}$

query: (h, r,?)

 $S_{\theta}(h,r,e)$ for all e in \mathcal{E}



$$MR = \frac{1}{Q} \sum_{i} rank_{i}$$

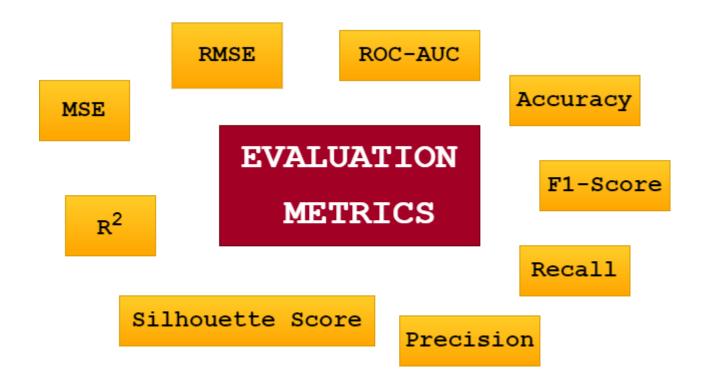
$$MRR = \frac{1}{Q} \sum_{i} 1/rank_{i}$$

$$Hits@k = \frac{1}{Q} \sum_{i} \mathbb{I}[rank_i \le k]$$

EVALUATION PROCEDURE



- The Judge : Metric
 - ☐ 'Which is the best model?'
 - ☐ Communities use conventional metrics according to the task environment

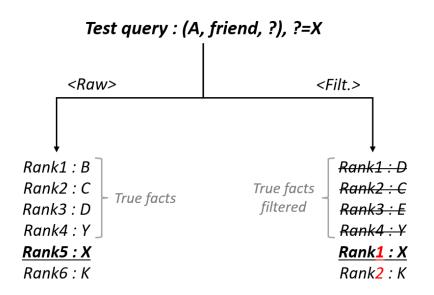


EVALUATION PROCEDURE

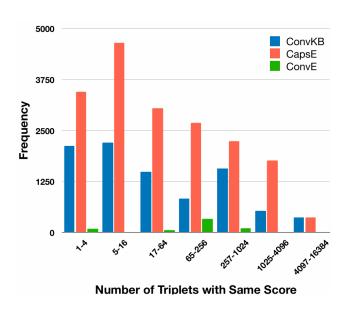


■ Flaws of Metrics & Protocols

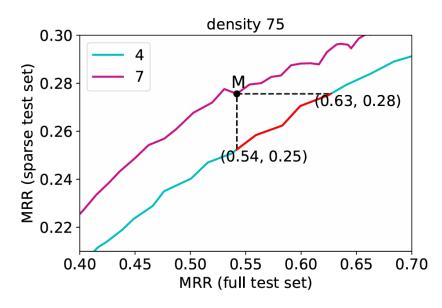
Filtered setting'13



Breaking ties'20



Open world problem'22



FILTERED SETTING



■ Translating Embeddings



Experiments

Conclusion



Translating Embeddings for Modeling Multi-relational Data

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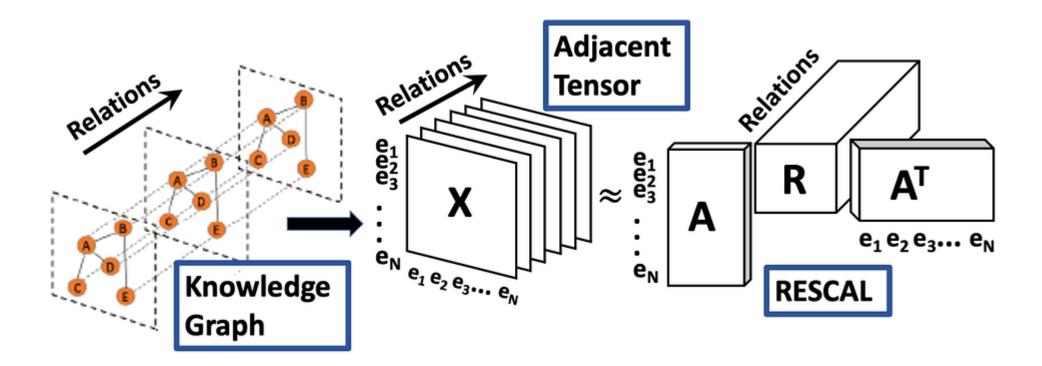
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TRANSLATING EMBEDDINGS



■ Tensor Factorization for KGC

- ☐ Popular approach for modeling multi-relational data
- ☐ Expensive model training (e.g., RESCAL)

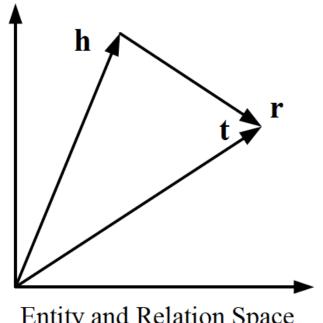


TRANSLATING EMBEDDINGS

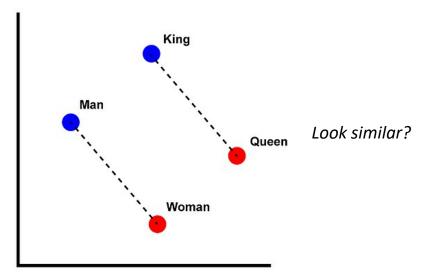


Simple Vector Addition

- ☐ View entity, relation as individual vector
- \square Optimize $m{h} + m{r} pprox m{t}$ for every triple in KG : "**Trans**lating **E**mbeddings"





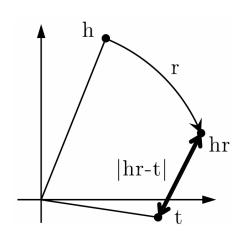


TRANSLATING EMBEDDINGS

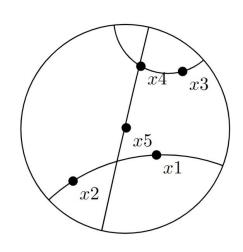


Revolutionized KGC

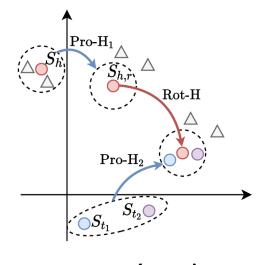
- ☐ Significant drop in training cost
- \square Simple design & mathematical motivation \rightarrow numerous extensions



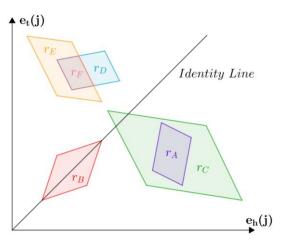
RotatE (2019)



MuRP (2019)



HousE (2022)



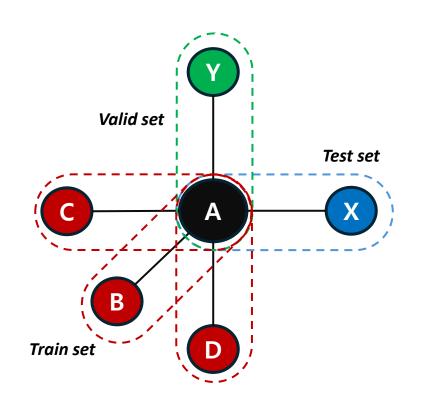
ExpressivE (2023)

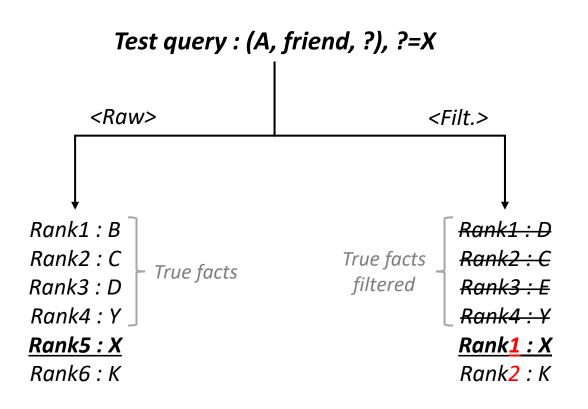
FILTERED SETTING



Introduction to Filtered Setting

☐ Raw : with out filtered setting, Filt. : with filtered setting





FILTERED SETTING



Experiment Results

DATASET		W	N			FB	15K		FB1M			
METRIC	MEAN RANK		HITS@	10 (%)	MEAN RANK		HITS@10 (%)		MEAN RANK	HITS@10 (%)		
Eval. setting	Raw	Filt.	Raw	Filt.	Raw	Filt.	Raw	Filt.	Raw	Raw		
Unstructured [2]	315	304	35.3	38.2	1,074	979	4.5	6.3	15,139	2.9		
RESCAL [11]	1,180	1,163	37.2	52.8	828	683	28.4	44.1	-	-		
SE [3]	1,011	985	68.5	80.5	273	162	28.8	39.8	22,044	17.5		
SME(LINEAR) [2]	545	533	65.1	74.1	274	154	30.7	40.8	-	-		
SME(BILINEAR) [2]	526	509	54.7	61.3	284	158	31.3	41.3	-	-		
LFM [6]	469	456	71.4	81.6	283	164	26.0	33.1	-	-		
TransE	263	251	75.4	89.2	243	125	34.9	47.1	14,615	34.0		

CONCLUSION

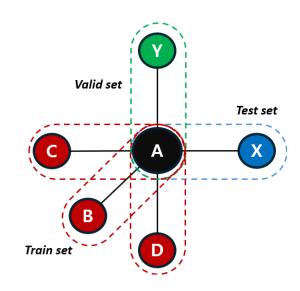


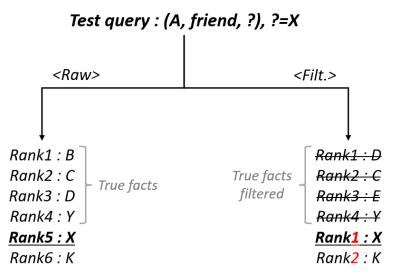
Simple yet Obvious

- ☐ Presence of external answers should not occupy rank position
- ☐ Simple yet obvious idea

Influence on the Community

- ☐ Became the 'default' protocol
- ☐ Main reason: 'no reason not to'





BREAKING TIES



- Background
- Problem Search

New Protocol

- Experiments
- Extended Discussion

Conclusion



A Re-evaluation of Knowledge Graph Completion Methods

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Partha Talukdar² Yiming Yang¹

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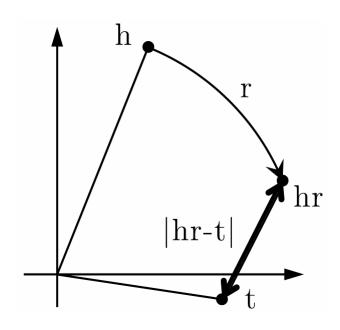
{zhiqings, svashish, yiming}@cs.cmu.edu

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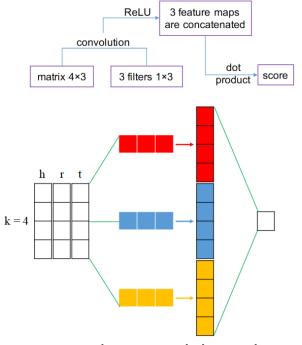


Many Types of KGC Models

□ SOTA KGC methods have been published in top conferences in recent years



Embedding based

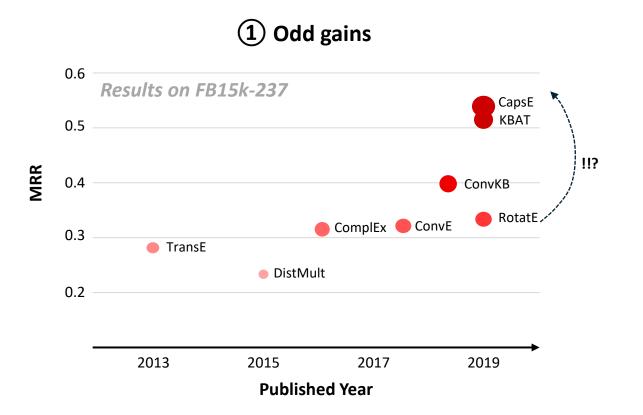


Neural Network based



Casting Doubt on Reported Results

- ☐ Several NN based models reported odd performance on FB15k-237 dataset
- ☐ Outlier performance **not consistent** across different datasets



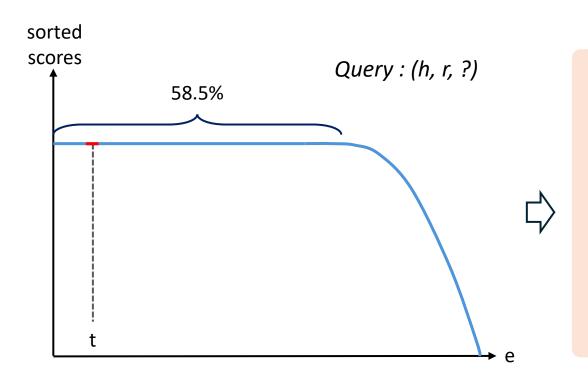
2 Inconsistency

	FB15k-237	WN18RR
ConvE	.325	.430
RotatE TuckER	.338 (+4.0%) .358 (+10.2%)	.476 (+10.6%) .470 (+9.3%)
ConvKB CapsE KBAT TransGate	.396 (+21.8%) .523 (+60.9%) .518 (+59.4%) .404 (+24.3%)	.248 (-42.3%) .415 (-3.4%) .440 (+2.3%) .409 (-4.9%)

PROBLEM SEARCH



■ (Obs.1) Too Many Same Scores



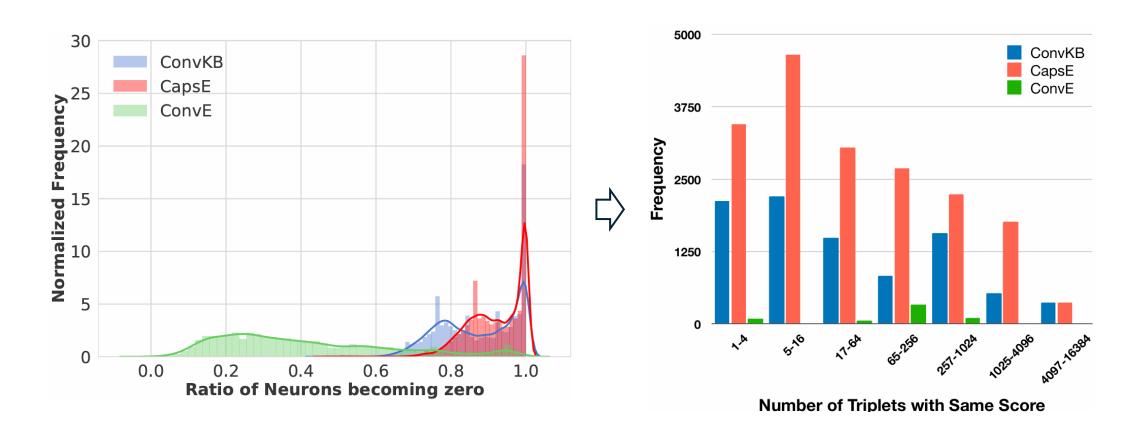
r(t) = count[score(e) > score(t)] + 1No discriminative power $r(t) = position_{score}[t]$ Dependent on the sorting algorithm

PROBLEM SEARCH



■ (Obs.2) Dead Neurons After Activation

 \square Reason for so many same scores ($\sigma = ReLU$)

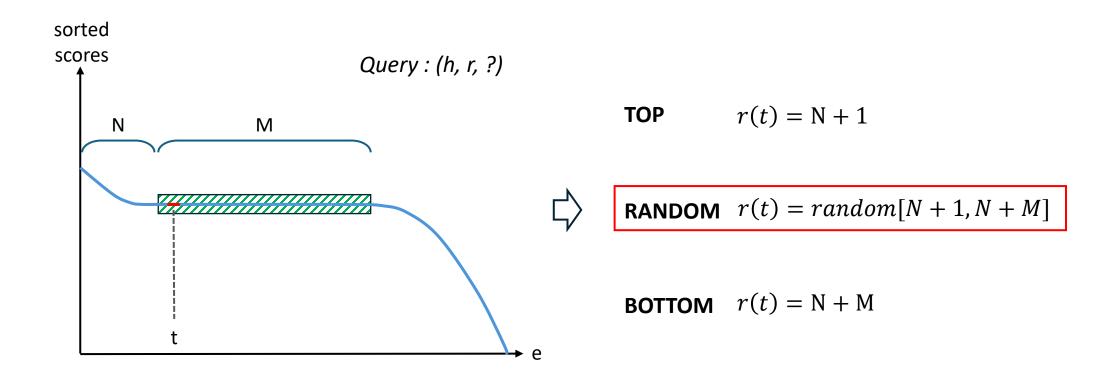


NEW PROTOCOL



■ Random Protocol for Tied Scores

☐ Models the realistic situation when ties occurred during knowledge extraction



EXPERIMENTS



■ FB15k237 : Random VS Top VS Bottom

	Reported				RANDOM	[Тор		Воттом			
	MRR ↑	MR ↓	H@10↑	MRR ↑	MR ↓	H@10↑	MRR ↑	MR↓	H@10↑	MRR ↑	MR ↓	H@10↑	
ConvE RotatE TuckER	.325 .338 .358	244 177 -	.501 .533 .544	$.336 \pm .0$	178 ± 0	$.501 \pm .0$ $.530 \pm .0$ $.536 \pm .0$.336	285 178 162	.501 .530 .536	.324 .336 .353	285 178 162	.501 .530 .536	
ConvKB	.396	257	.517	$.243 \pm .0$	309 ± 2	.421 ± .0	.407 (+.164)	246 (-63)	.527 (+.106)	130 (113)	373 (+64)	.383 (038)	
CapsE	.523	303	.593	$.150 \pm .0$	403 ± 2	$.356 \pm .0$.511 (+.361)	305 (-99)	.586 (+.229)	134 (016)	502 (+99)	.297 (059)	
KBAT	.518†	210†	.626†	$.157 \pm .0$	270 ± 0	$.331 \pm .0$.157	270	.331	.157	270	.331	

^{*}KBAT reimplemented due to test data leakage

EXPERIMENTS



■ WN18RR: Random VS Top VS Bottom

]	Report	ed		RANDOM			Тор		Воттом			
	MRR ↑	MR↓	H@10↑	MRR ↑	MR↓	H@10↑	MRR ↑	MR ↓	H@10↑	MRR ↑	MR↓	H@10↑	
ConvE RotatE TuckER	.43 .476 .470	4187 3340 -	.52 .571 .526	$.473 \pm .0$	4950 ± 0 3343 ± 0 6324 ± 0	$.571 \pm .0$.473	4950 3343 6324	.503 .571 .516	.444 .473 .461	4950 3343 6324	.503 .571 .516	
ConvKB	.248	2554	.525	.249 ± .0	3433 ± 42	.524 ± .0	.251 (+.002)	1696 (-1737)	.529 (+.005)	164 (085)	5168 (+1735)	.516 (008)	
CapsE‡	.415	719	.560	$.415 \pm .0$	718 ± 0	$.559 \pm .0$.415	718	.559	323 (092)	719 (+1)	.555 (004)	
KBAT	.440†	1940†	.581†	$.412 \pm .0$	1921 ± 0	$.554 \pm .0$.412	1921	.554	.412	1921	.554	

^{*}KBAT reimplemented due to test data leakage

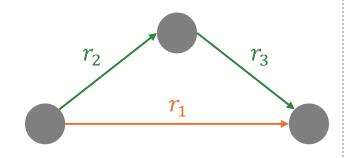
EXTENDED DISCUSSION



Potential Problem : Rule-Based Model

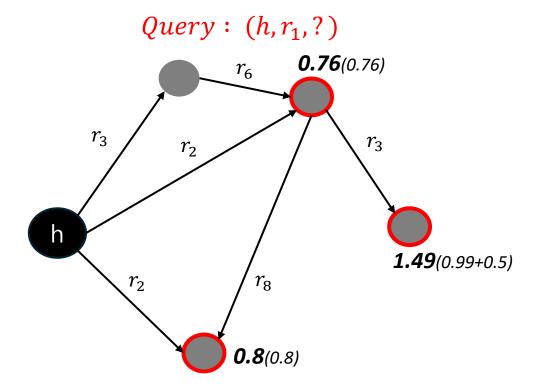
head

: [body] (confidence)



Mined rules

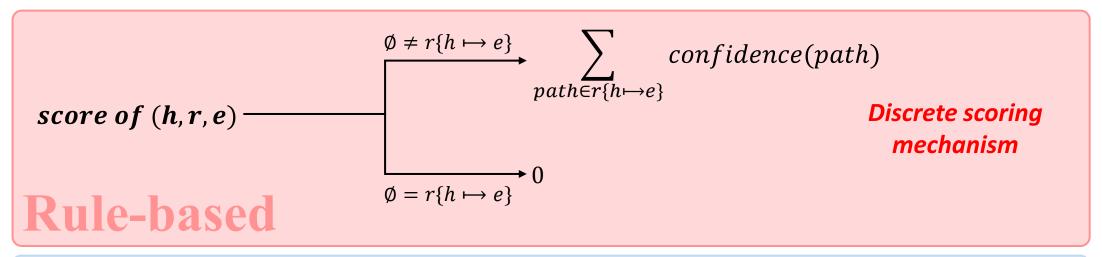
$$\begin{bmatrix} r_1: r_2 \to r_3 \ (0.99) \\ r_1: r_2 \to r_8 \ (0.8) \\ r_1: r_3 \to r_6 \ (0.76) \\ r_1: r_3 \to r_6 \to r_3 \ (0.5) \\ r_1: r_4 \to r_3 \ (0.1) \\ r_2: r_1 \to r_2 \to r_3 \ (0.8) \\ r_2: r_1 \to r_3 \ (0.6) \\ \vdots$$

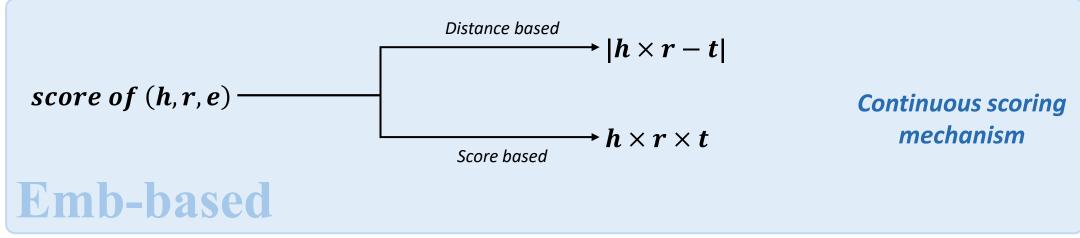


EXTENDED DISCUSSION



Potential Tied Scores





EXTENDED DISCUSSION



Gap Between Reported Results of Rule-Based Models

Mathad			Fan	nily			Kins	ship			UM	ILS			WN1	18RR			FB15l	k-237			YAGO	03-10	
Method	MRI	?]	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10												
TransE [†]	0.45	0 2	22.1	-	87.4	0.310	0.9	-	84.1	0.690	52.3	-	89.7	0.230	2.2	-	52.4	0.294	18.9	-	46.5	0.360	25.1	-	58.0
DistMult [†]	0.54	0 3	36.0	-	88.5	0.354	18.9	40.0	75.5	0.391	25.6	44.5	66.9	0.430	39.0	44.0	49.0	0.241	15.5	26.3	41.9	0.340	24.3	-	53.3
ComplEx [†]	0.81	0 7	72.7	-	94.6	0.418	24.2	49.9	81.2	0.411	27.3	46.8	70.0	0.440	41.0	46.0	51.0	0.247	15.8	27.5	42.8	0.340	24.8	-	54.9
ConvE [†]	-		-	-	-	-	-	-	-	-	-	-	-	0.430	40.0	44.0	52.0	0.320	21.6	-	50.1	0.440	35.5	-	61.6
R-GCN [†]	-		-	-	-	-	-	-	-	-	-	-	-	0.402	34.5	43.7	49.4	0.273	18.2	30.3	45.6	-	-	-	-
TuckER [†]	-		-	-	-	0.630	46.2	69.8	86.3	0.732	62.5	81.2	90.9	0.470	44.3	48.2	52.6	0.358	26.6	39.4	54.4	-	-	-	-
RotatE [†]	0.86	0 7	78.7	-	93.3	0.651	50.4	75.5	93.2	0.744	63.6	82.2	93.9	0.476	42.8	49.2	57.1	0.338	24.1	37.5	53.3	0.490	40.2	-	67.0
AMIE+ [†]	0.54	1 4	48.7	59.2	59.6	0.416	23.7	49.3	83.0	0.417	25.3	51.9	68.5	0.192	19.0	19.5	19.6	0.118	8.8	13.1	17.3	0.259	23.1	28.4	30.3
MLN^{\dagger}	-		-	-	-	0.351	18.9	40.8	70.7	0.688	58.7	75.5	86.9	-	-	-	-	-	-	-	-	-	-	-	-
Path $Rank^\dagger$	-		-	-	-	0.369	27.2	41.6	67.3	0.197	14.8	21.4	25.2	0.189	17.1	20.0	22.5	0.087	7.4	9.2	11.2	-	-	-	-
NeuralLP [†]	0.88	0 8	80.1	-	98.5	0.302	16.7	33.9	59.6	0.483	33.2	56.3	77.5	0.381	36.8	38.6	40.8	0.237	17.3	25.9	36.1	-	-	-	-
DRUM^\dagger	0.89	0 8	82.6	-	99.2	0.334	18.3	37.8	67.5	0.548	35.8	69.9	81.4	0.382	36.9	38.8	41.0	0.238	17.4	26.1	36.4	-	-	-	-
$NLIL^\dagger$	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.250	-	-	32.4	-	-	-	-
CTP^\dagger			-	-	-	0.335	17.7	37.6	70.3	0.404	28.8	43.0	67.4	-	-	-	-	-	-	-	-	-	-	-	-
RLogic [†]	0.88	0 8	81.3	-	97.2	0.580	43.4	-	87.2	0.710	56.6	-	93.2	0.470	44.3	-	53.7	0.310	20.3	-	50.1	0.360	25.2	-	50.4
NCRL*	0.91	0 8	85.2	-	99.3	0.640	49.0	-	92.9	0.790	65.9	-	95.1	0.670	56.3	-	85.0	0.300	20.9	-	47.3	0.380	27.4	-	53.6
NCRL^\dagger	0.80	6	74.0	86.0	90.1	0.537	38.6	62.6	83.4	0.562	45.9	61.6	71.5	0.263	23.2	28.0	31.3	0.141	7.5	17.0	26.6	0.012	0.3	1.3	2.8
RNNLogic [†]	0.86	0 7	79.2	-	95.7	0.639	49.5	73.1	92.4	0.745	63.0	83.3	92.4	0.455	41.4	47.5	53.1	0.288	20.8	31.5	44.5	0.379	30.2	42.1	53.3
TCLM [†]	0.98	5 9	98.1	98.9	99.1	0.686	54.3	79.5	95.3	0.808	73.0	87.1	92.8	0.483	44.7	49.7	55.2	0.311	23.0	34.0	47.2	0.505	43.4	54.7	63.5
TCLM (w/o IC)	0.98	4 9	97.9	98.9	99.0	0.684	54.1	79.1	95.1	0.788	70.0	86.2	92.8	0.462	42.7	47.6	53.6	0.309	22.8	33.8	46.7	0.430	34.3	47.4	59.1

CONCLUSION



Subtle yet Crucial

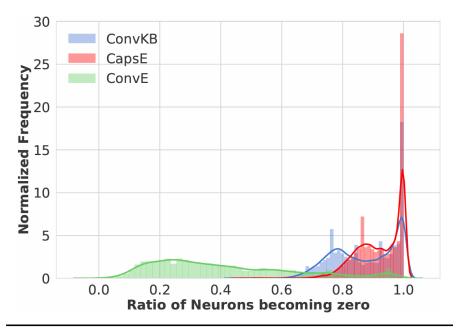
□ Observed anomalous metric results

Finding the Cause & Remedy

- ☐ Rank ties resulting in metric inflation
- ☐ Random protocol for reasonable evaluation

Influence on the Community

- ☐ Quite recognized among researchers
- □ Not fully adopted compared to the filtered setting



]	Reporte	ed	RANDOM								
	MRR ↑	MR ↓	H@10↑	MRR ↑	MR ↓	H@10↑						
ConvE	.325	244	.501	$.324 \pm .0 $	285 ± 0	$.501 \pm .0$						
RotatE	.338	177	.533	0.336 ± 0.0	178 ± 0	$.530 \pm .0$						
TuckER	.358	-	.544	$353 \pm .0$	162 ± 0	$.536 \pm .0$						
ConvKB	.396	257	.517	$243 \pm .0$	309 ± 2	.421 ± .0						
CapsE	.523	303	.593	$1.150 \pm .0$	403 ± 2	$.356 \pm .0$						
KBAT	.518†	210†	.626†	$.157 \pm .0 $	270 ± 0	$.331 \pm .0$						

THE OPEN WORLD



Background

Problem Definition

■ Theoretical Approach

Experiments

Discussion



Rethinking Knowledge Graph Evaluation Under the Open-World Assumption

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Inherent and Philosophical Question









fact not present → fact false

system's knowledge is <u>complete</u> = the world is <u>closed</u>

Closed World Assumption



Inherent and Philosophical Question



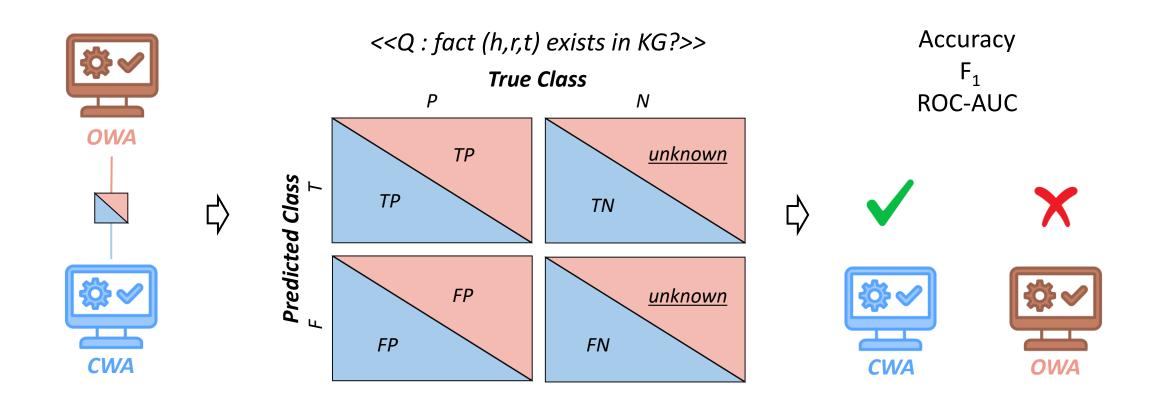
fact not present → fact unknown

system's knowledge is <u>incomplete</u> = the world is <u>open</u>

Open World Assumption



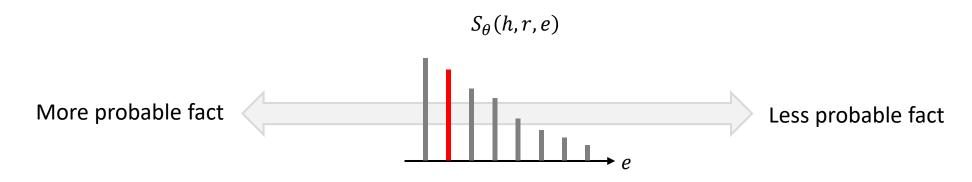
Crucial Definition Before Evaluation





Rank-Based Metrics

- ☐ FN/TN not required
- ☐ Only interested in putting true positives in front of unknowns



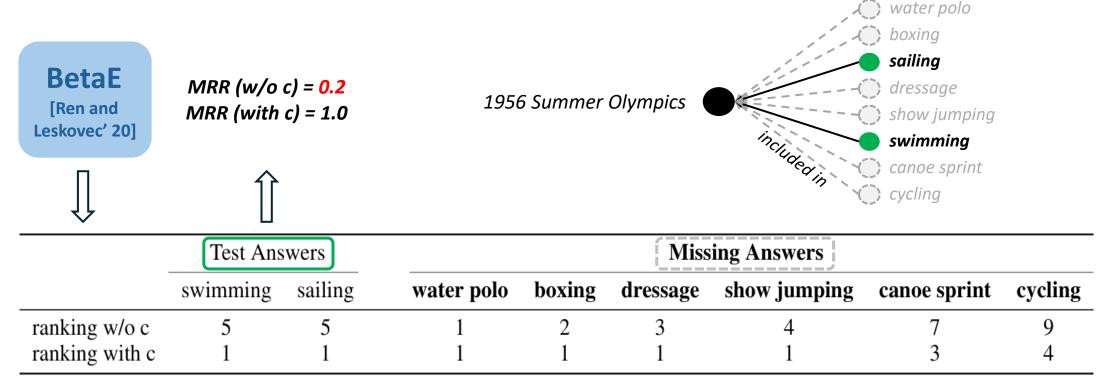
■ KGC and Rank-Based Metrics

- ☐ Finding new knowledge = KGC's main purpose → KGC follows OWA
- ☐ Exclusive use of rank-based metrics (MR, MRR, Hits@k)



Problem with Missing Answers

□ (?, included in, 1965 Summer Olympics); existing answers = swimming, sailing

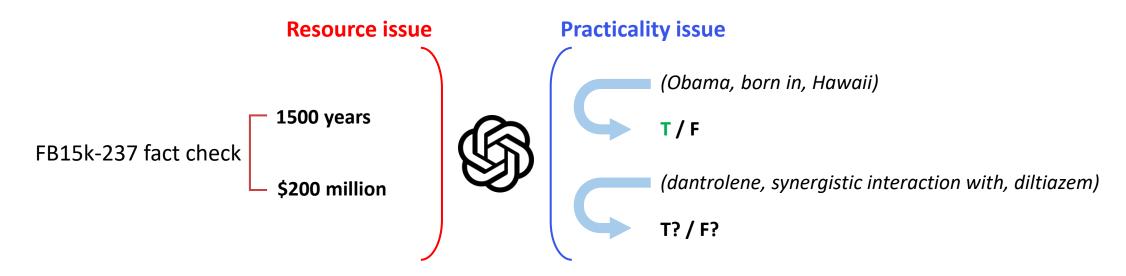


w/o c : with out correction, with c : with correction



Alleviating the Sparsity

☐ Augmentation via Gen-AI : feasible? **No**

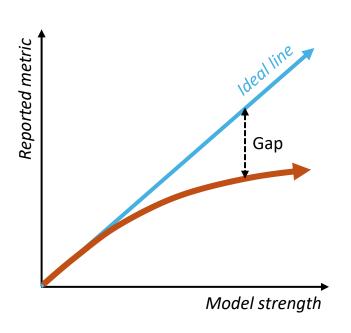


	FB15k-237	WN18RR	YAGO3-10	DDB14	Hetionet
$\overline{ E }$	14541	40943	123182	9203	45158
R	237	11	37	14	23
$ E ^2 R $	50B	18B	561B	1B	47B

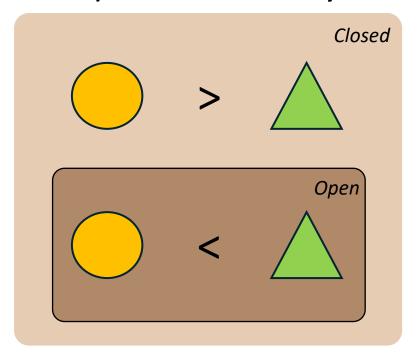


■ Two Problems Affecting the KGC Evaluation

1) Metric degradation



2) Metric inconsistency





■ The Ultimate Question

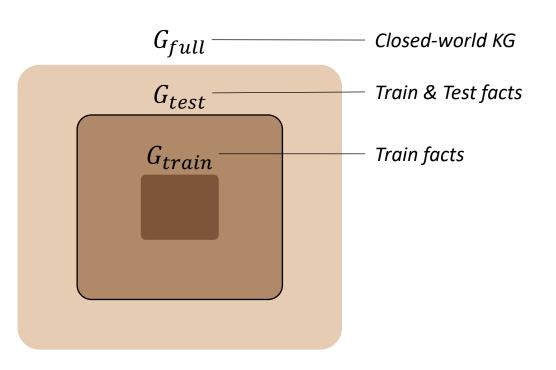
Full test facts

Sparse test facts

 $G_{full} \setminus G_{train}$

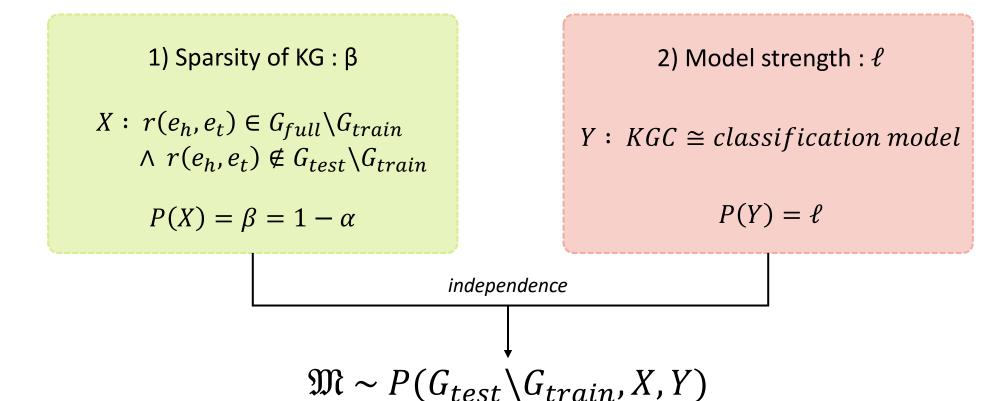
 $G_{test} \backslash G_{train}$

"Are evaluation from sparse test facts and full test facts consistent?"





■ Two Source of Randomness





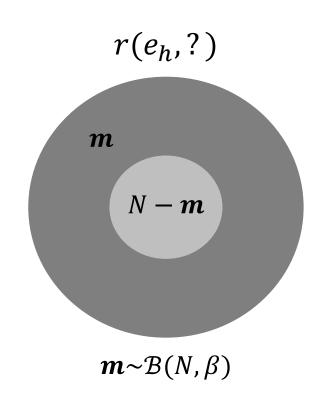
Expectation Degradation

$$MRR: f(r) = r$$

Hits@k:
$$f(r) = 1$$
 if $r \le k$ else ∞

$$\mathfrak{M} = \frac{1}{N-m} \sum_{i=1}^{N-m} \frac{1}{f(\mathbf{r}(e_i))}$$

$$\hat{\mathbb{E}} = \mathbb{E}(\mathfrak{M}) = \frac{1}{\beta(N+1)} \sum_{k=0}^{N} \frac{1}{f(k+1)} \left(1 - \hat{\Phi}(k) \right)$$



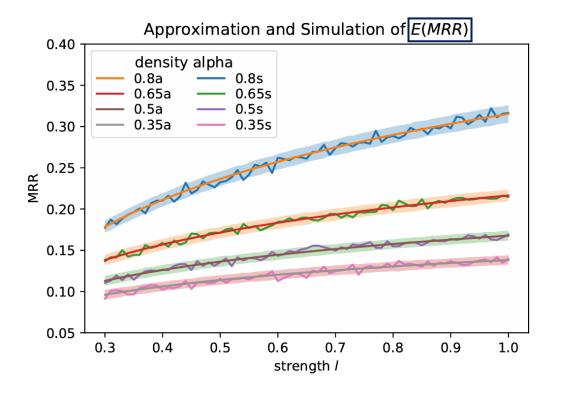
38



Expectation Degradation

$$\hat{\mathbb{E}}(MRR) \approx \frac{\ln(\ell) + \ln(\beta) + \ln(N+2) + \gamma}{\beta(N+1)} := \tilde{\mathbb{E}}$$

- ◆ MRR will behave like a log function w.r.t the growth of ℓ
- ◆ Perfect model can't achieve MRR=1 due to sparsity β





Inconsistency Due to High Variance

$$\mathcal{M}_1 = \ell$$
 $\mathcal{M}_2 = \ell + \Delta \ell$

$$P[\mathfrak{M}(\mathcal{M}_1) \geq \mathfrak{M}(\mathcal{M}_2)] \xrightarrow{\mathsf{reject}} N_q \geq \mathcal{O}((1/\Delta\ell)^2)$$

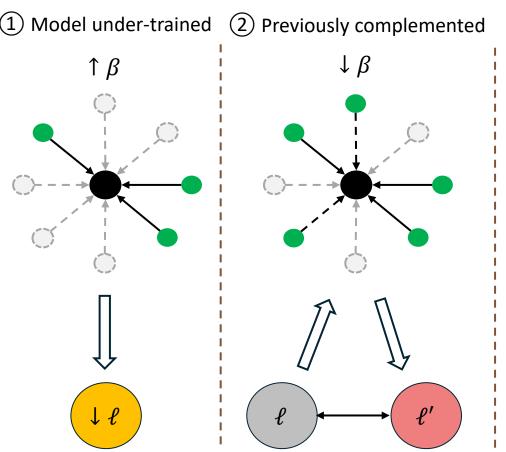
of test queries quadratically grows w.r.t $1/\Delta \ell$



Close model strengths demand <u>cautious comparison</u>



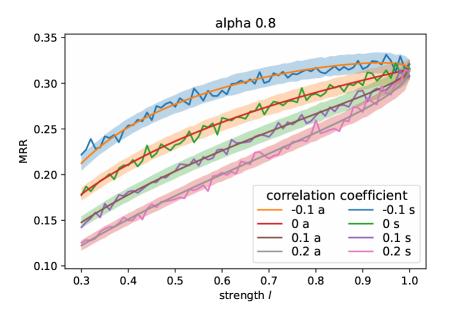
lacksquare Considering Correlation Between eta and $oldsymbol{\ell}$



Negative correlation between $oldsymbol{eta}$ and $oldsymbol{\ell}$

According to Corollary 4.5 in the paper, MRR favor models with smaller ho instead of larger $m{\ell}$

More severe inconsistency!!!





Need for New Metric

 \square The only changeable element : transform function f, but how?

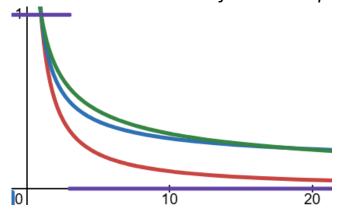


- $\blacksquare | \operatorname{Hits@k} : f(r) = \mathbb{I}[r \le k]$
- $\log MRR : f(r) = \log_2(r+1)$
- p-MRR : $f(r) = r^p (0$

Less focus-on-top



$$\frac{\mathrm{d}\hat{\mathbb{E}}(\mathfrak{M})}{\mathrm{d}\ell} = \frac{1}{l\beta(N+1)} \, \mathbb{E}_{k \sim \mathcal{B}(N+1,\ell\beta)} \, g(k)$$



 \downarrow focus-on-top $\rightarrow \downarrow$ degradation & \downarrow inconsistency

More credibility to the conclusion



Dataset, Models, Metrics Setup

Family-tree		Dataset
# entities	6004	➤ Closed-world
# relations	23	► Sparsity controllable
# facts	192,532	

Focus-on-top

MRR

VS

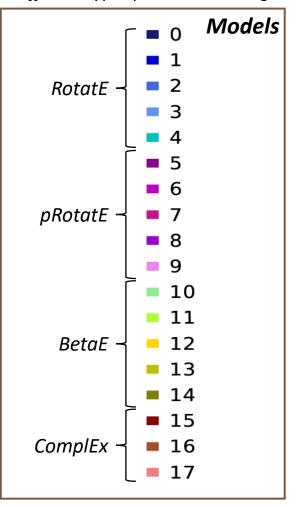
log-MRR

Hits@1, 3, 10

P-MRR

- ► Metric degradation & inconsistency w.r.t sparsity
- ► Effect of new metric
- \blacktriangleright Under the dependency assumption between $\beta \& \ell$

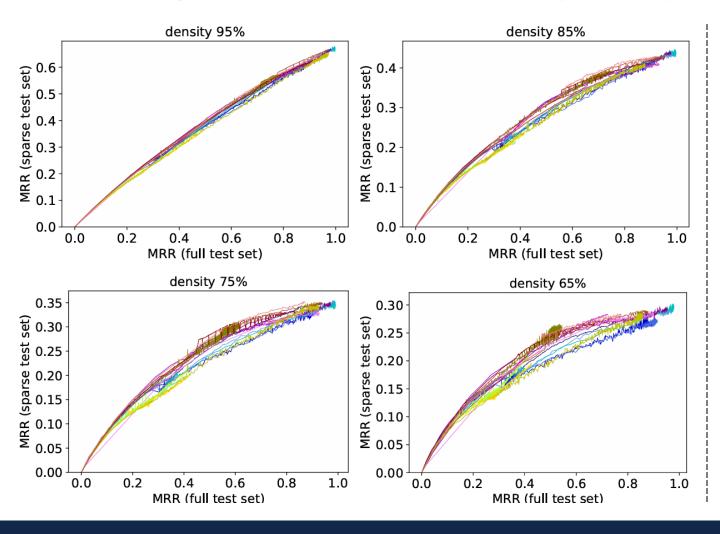
*different hyper-parameter settings

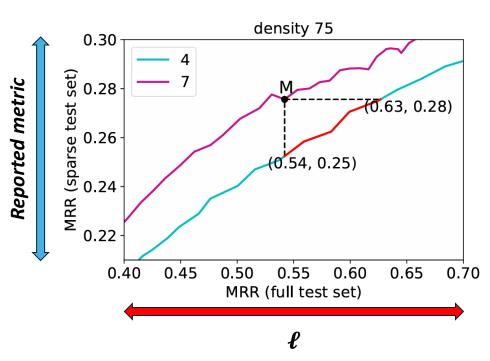


Goal



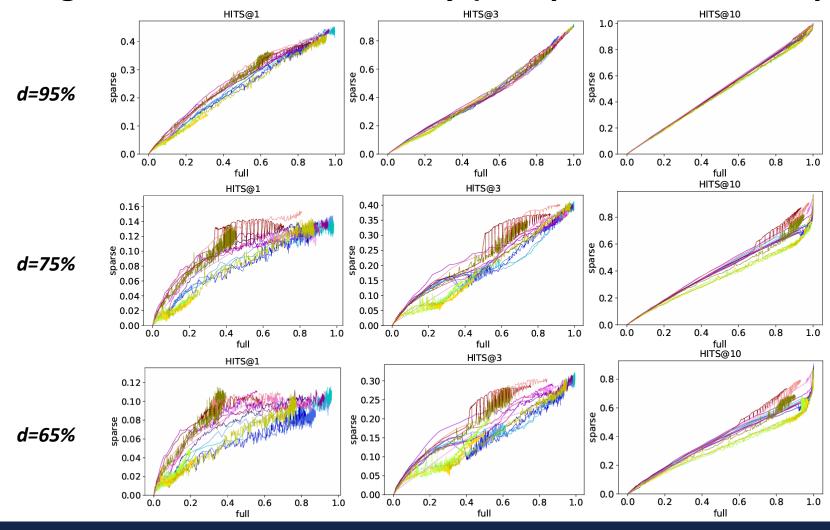
MRR Degradation & Inconsistency (Independence Assumption)





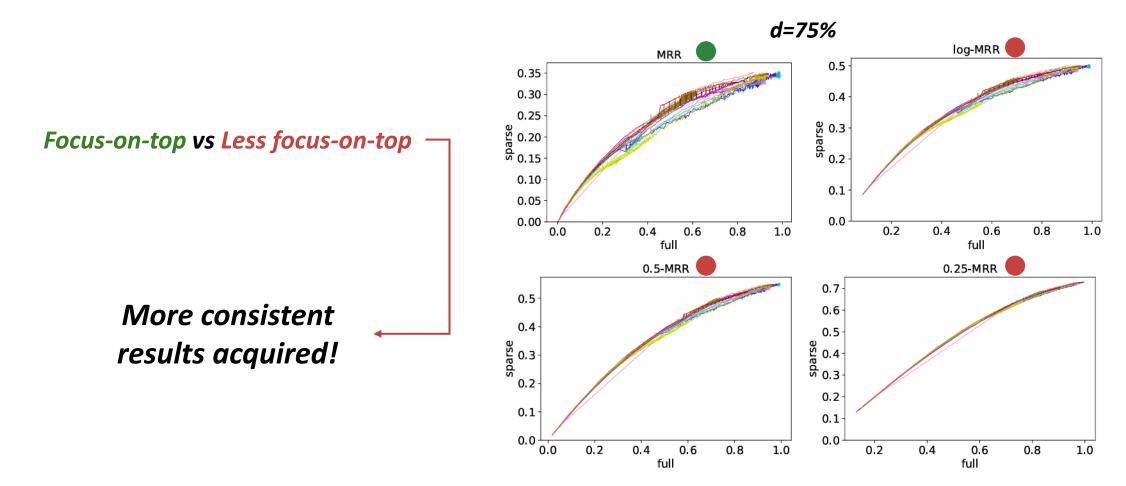


Hits@k Degradation & Inconsistency (Independence Assumption)





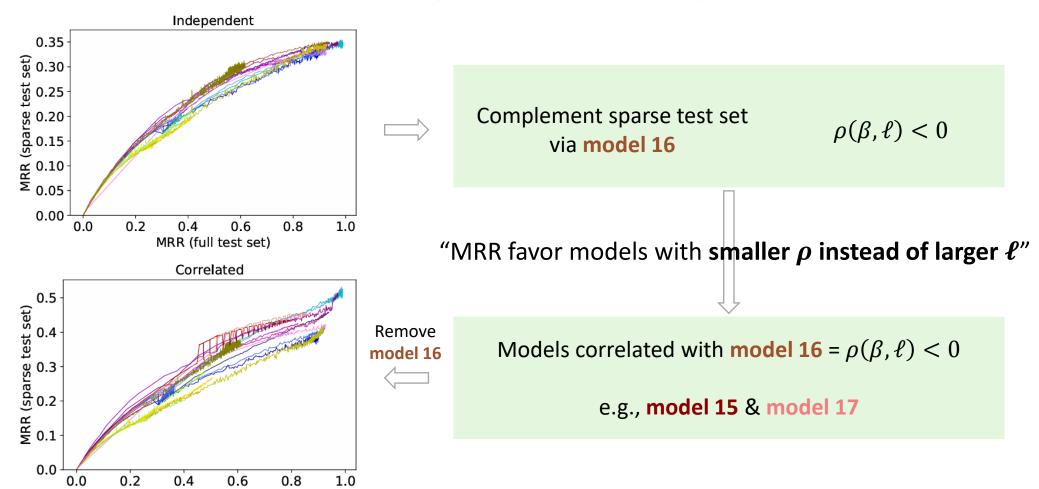
Alleviating Degradation and Inconsistency (Independence Assumption)

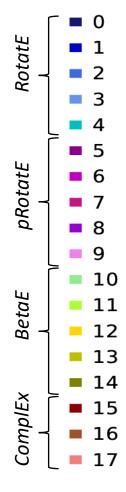


MRR (full test set)



Presence of Correlation (Dependence Assumption)



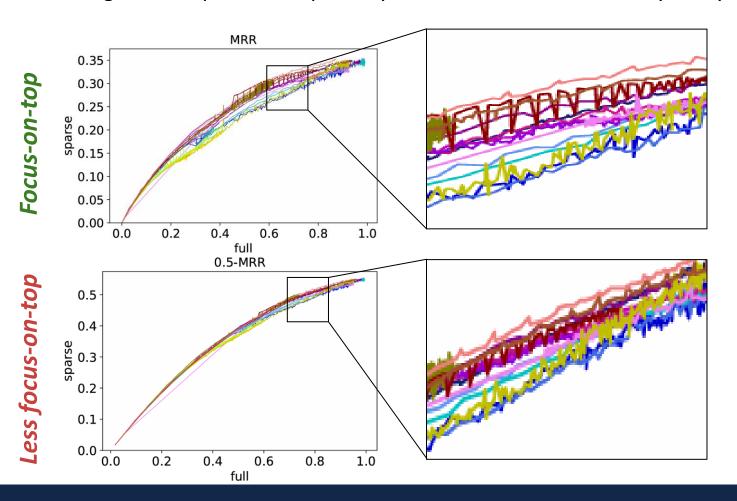


DISCUSSION



■ Illusion of Less Focus-on-Top?

☐ Degradation problem is partially solved / is the inconsistency really alleviated?



Squeezed values of LFOT

- → smaller difference
- → illusion of consistency

The most ideal metric in terms of less degradation & consistency = $1/r^p(p \rightarrow 0)$ \rightarrow values collapse closer to each other

CONCLUSION



Discussion on Innate Trate of Open World Graph

- ☐ Theoretical investigation
- ☐ Metric's interpretation on model strength given sparsity

Metric Degradation & Inconsistency

- ☐ Acknowledging limitations of conventional metrics
- ☐ Proved via experiments

New Metrics

- ☐ Proposing less focus-on-top metrics
- ☐ Validated experimentally

