CRule: Category-Aware Symbolic Multi-Hop Reasoning on Knowledge Graphs

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Abstract—
Multi-hop reasoning is essential in knowledge graph (KG) research and applications. Current methods rely on specific KG entities, while human cognition operates at a more abstract level. This paper proposes a Category-aware Rule-based (CRule) approach for symbolic multi-hop reasoning. Specifically, given a KG, CRule first categorizes entities and constructs a category-aware KG, then uses rules retrieved from the categorized KG to perform multi-hop reasoning on the original KG. Experiments on five datasets show that CRule is simple, effective, and combines the advantages of symbolic and neural network methods. It overcomes symbolic reasoning's complexity limitations, can perform reasoning on KGs of more than 300k edges, and can be three times more efficient than neural network models.

Introduction

Multi-hop reasoning infers missing knowledge based on paths in KGs. For example, query (Athlete_Albert_Pujols, AthletePlaysforTeam, ?) aims to find the missing entity with relation "AthletePlaysforTeam" to entity "Athlete_Albert_Pujols". Multi-hop reasoning finds the missing entity by following path "Athlete_Albert_Pujols $\xrightarrow{\text{AthleteHomeStadium}}$ busch_memorial_stadium $\xrightarrow{\text{TeamHomeStadium\_inv}}$ Sportsteam_St_Louis_Cardinals", which is semantically equal to "Athlete_Albert_Pujols $\xrightarrow{\text{AthletePlaysforTeam}}$ Sportsteam_St_Louis_Cardinals". Multi-hop reasoning provides a higher level of interpretability when compared to embedding-based reasoning, and is often employed in scenarios such as query answering.

While current multi-hop reasoning methods rely on concrete entities, human cognition operates at a more abstract level, as demonstrated by the salience of categories aiding abstract thinking [1]. A category refers to a mental representation of a group of objects, ideas, or events sharing common features. Categories play a crucial role in human cognition by facilitating various cognitive processes, including organizing and structuring knowledge, forming abstract concepts through instance grouping, enabling generalization and inference about unfamiliar instances, and more. Therefore, it is crucial to investigate how to automatically abstract entities into categories and perform category-based reasoning.

In this paper, we simulate the cognitive process of categorization, construct a category-aware KG, and propose a corresponding symbolic multi-hop reasoning model, CRule. We utilize the "1-

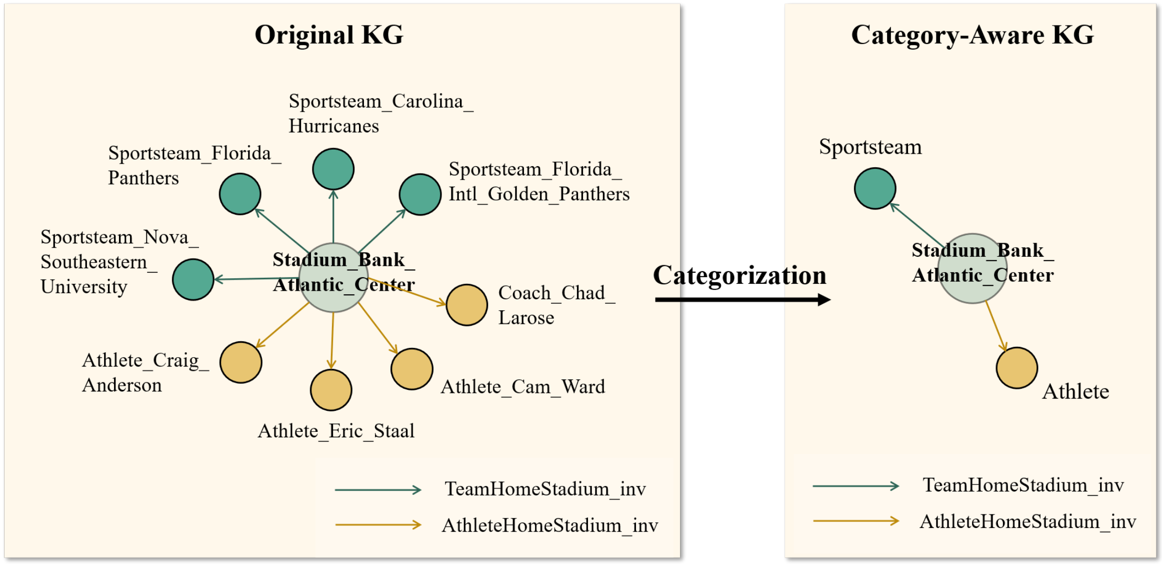

Figure 1: Example of categorization. Tail entities share the same relation with the same head entity fall under one category. "Sportsteam" and "Athlete" are two categories in the category-aware KG.

Table 1: Comparison of symbolic methods, NN-based methods and CRule, where "NN" refers to "neural network". Green marks the strengths of the model while red marks the weaknesses.

	Symbolic Methods	NN-Based Methods	CRule
Reasoning Performance	Poor	Good	Good
Applicability on Large KGs	Poor	Good	Good
Computing Resource Demand	Low	High	Low
Hypermeter-Tuning Demand	Low	High	Low
Model-Training Demand	Low	High	Low

N" structure to construct categories, where a single head entity and relation are associated with multiple tail entities. In such cases, the tail entities can be considered as having the same properties, and therefore belong to the same category. As shown in Fig. 1, multiple entities have relations "TeamHomeStadium_inv" with entity "Stadium_Bank_Atlantic_Center", all of them belong to the category "Sportsteam". A category-aware KG is built by connecting these categories. We extract rules and weights based on the categorized KG, finding missing entities by applying these rules to the original KG.

We use five datasets to evaluate model performance, including two small datasets and three large datasets. Experiments demonstrate that CRule can effectively generalize across datasets of varying scales. Additionally, it can integrate the advantages of existing methods, as shown in Table 1. It overcomes the disadvantages of neural network methods, which require high-performance computing resources, long training time, and careful parameter tuning, while also addressing the scalability limitations of symbolic methods [2].

Our contributions are listed as follows:

- We propose a simple yet effective categorization method that can automatically form categories and construct category-aware KGs;
- We propose a symbolic reasoning method CRule based on the categorized KG, which can achieve good performance on datasets of varying sizes;
- CRule has the advantages of both symbolic and neural network methods, enabling high-quality reasoning performance while being training-free and non-parametric. Furthermore, it can also be applied to large-scale KGs with signif-

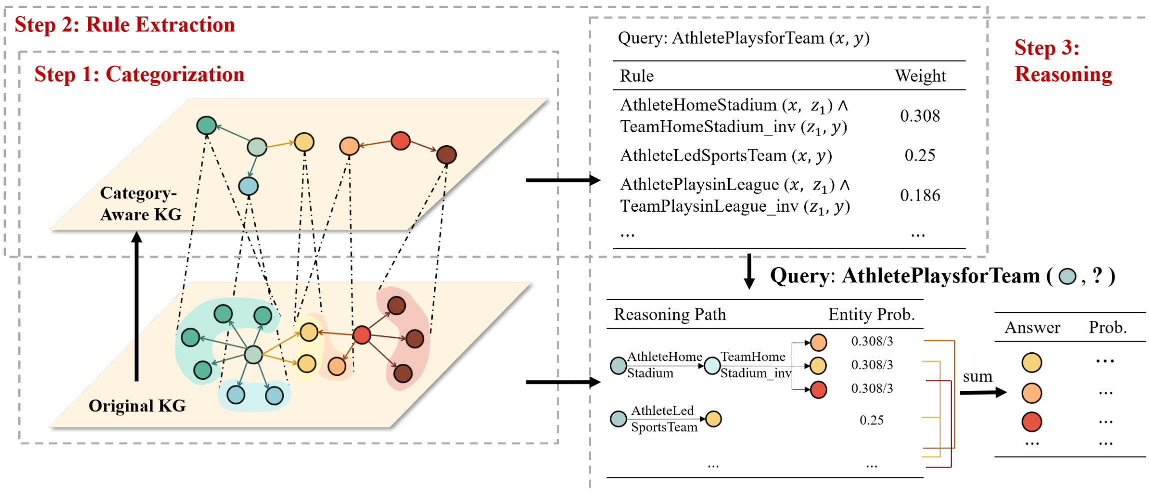

Figure 2: Overall structure of CRule. It first constructs a category-aware KG, then extracts rules based on it, finally reasons based on the extracted rules and the original KG.

icant improvements in reasoning efficiency.

Background

Problem Formulation

A KG is a set of triples, denoted as $\mathcal{G} = \{(h, r, t)\} \in \mathcal{E} \times \mathcal{R} \times \mathcal{E}$, where $\mathcal{E}$ is the entity set, $\mathcal{R}$ is the relation set, entities $h, t \in \mathcal{E}$, and relation $r \in \mathcal{R}$. A triple (h, r, t) denotes that head entity h and tail entity t have relation r.

Multi-hop reasoning on KGs seeks to answer queries in form $(h, r, ?)$, that is, finding entities that have relation r with entity h, by identifying paths starting from h with semantics equivalent to relation r. This paper aims to automate the categorization of entities and implement multi-hop reasoning based on the categorized KG.

Related Work

KG reasoning differs from rule mining in other research domains like data profiling. In data profiling, rule mining focuses on extracting association rules, while KG reasoning aims to discover first-order predicate logic rules. KG reasoning involves a wider variety of relations and more complex rules types.

For KG reasoning, existing multi-hop reasoning methods rely on specific entities, including symbolic-based methods and neural network-based methods.

Symbolic multi-hop reasoning methods, such as AMIE [3], performs reasoning based on extracted rules. When dealing with large-scale KGs, however, it suffers from enormous complexity and inefficiency. RuleN [4] addresses this problem by sampling and using only part of the KGs, thus sacrifices some effectiveness. Most of the current symbolic reasoning methods deal with this issue by combining with machine learning techniques or neural networks, such as PRA [5], MLN [6], and Neural LP [7]. These methods are less effective in reasoning compared to neural network methods.

Due to the complexity limitation and poor performance of symbolic methods, current mainstream methods are based on neural networks. RNN-Chains [8] models the reasoning paths as text sequences, and finds the target entities based on the paths' semantics; DeepPath [9], MINERVA [10], Multihop-KG [11], and [12] utilize reinforcement learning to identify missing entities by searching for paths within KGs. Although these methods can be applied to large-scale KGs with better results, they are more computationally demanding, require carefully tuned parameters and long training time.

KG reasoning can also be realized using single-hop representation learning methods such as TransE [13], TransR [14], DistMult [15], ComplEx [16], ConvE [17], and GIE [18]. However, such methods only use single triples instead of paths, resulting in a lack of interpretability when compared to multi-hop reasoning approaches.

Methodology

This section describes our method. Fig. 2 illustrates the structure of the proposed CRule.

Categorization

Category Generation. Based on the given KG, for query $(h, r, ?)$, we consider all the satisfied tail entities belonging to the same category, denoting as h_r. Note that each entity may be involved in multiple "1-N" relations, thus one entity can fall into several different categories.

Category-Aware KG. We then construct the category-aware KG by mapping the original entities to the generated categories. Specifically, for a triple (h, r, t), we replace its head entity h with all category nodes to which h belongs; for the tail entity t, we substitute it with the category node h_r; then, all those head category nodes and tail category node h_r are connected by relation r.

Rule Extraction

To implement symbolic reasoning, we mainly extract symbolic rules based on the constructed category-aware KG, and supplement them with rules from the original KG.

For a query relation R, we first find the shortest path between categories of h and t in the category-aware KG, if no such path found, then we find the shortest path between entities h and t in the original KG instead. A rule ℓ is in form

$$R_1(x, z_1) \wedge R_2(z_1, z_2) \wedge \cdots \wedge R_n(z_{n-1}, y) \rightarrow R(x, y), \quad (1)$$

where x, y, z_n denotes categories or entities, $R(x, y)$ denotes x and y have relation R. Rule (1) indicates that x and y have relation R when path "$x \xrightarrow{R_1} z_1 \xrightarrow{R_2} z_2 \cdots z_{n-1} \xrightarrow{R_n} y$" exists. In this paper, we only focus on the relation chain "$R_1 \wedge R_2 \wedge \cdots \wedge R_n \rightarrow R$" and ignore categories and entities in rule extraction. The frequencies of rules are considered as their weights.

To further enhance the efficiency, we also propose a simplified setting that ignores cycles consisting of a relation and its inverse. For example, "$R_1 \wedge R_2 \wedge R_3$" is simplified to "$R_3$" if R_1 and R_2 are inverse to each other. This setting is denoted as CRule(s).

Reasoning

After getting rules, we perform reasoning on the original KG. For a query $(h, r, ?)$, we first identify the tail entities and their weights corresponding to each rule, then calculate the likelihood of candidate entities based on their weights.

For a rule ℓ "$R_1 \wedge R_2 \wedge R_3$", if there is a path "$h \xrightarrow{R_1} z_1 \xrightarrow{R_2} z_2 \xrightarrow{R_3} t$" in the original KG, then t is a candidate tail entity, with weight equals to the weight of ℓ multiplied by probabilities of choosing z_1, z_2 and t. The probability of choosing an entity is determined by the total number of candidates while choosing. Take z_1 as an example, if there are N entities satisfy $(h, R_1, ?)$, then the probability of choosing z_1 is $1/N$. Each candidate tail entity t's weight ω_t is calculated as

$$\omega_t = \sum_{\ell_i \in \mathcal{L}} \prod_{e_j \in \ell_i} \omega_{\ell_i} \omega_{e_1}^{\ell_i} \omega_{e_2}^{\ell_i} \cdots \omega_{e_{|\ell_i|+1}}^{\ell_i}, \quad (2)$$

where ω_{ℓ_i} denotes the weight of rule ℓ_i, $\mathcal{L}$ denotes the set of all rules, $\omega_{e_j}^{\ell_i}$ denotes the probability of choosing the j-th entity e_j under rule ℓ_i. Then for entity t, ω_t equals the sum of all its weights get from different rules.

The whole algorithm is shown in Algorithm 1.

Experiments and Results

In this section, we evaluate the performance of CRule and CRule(s).

Datasets

We evaluate the model using five datasets, including two small datasets, Countries [19] and Grid-World [7], and three large datasets, WN18RR [17], NELL-995 [9], and FB15k-237 [20]. Statistics of the datasets are shown in Table 2.

Table 2: Dataset statistics.

Dataset	$\lvert\mathcal{E}\rvert$	$\lvert\mathcal{R}\rvert$	#Triples
Countries	272	2	1,158
Grid-World	256	8	7,440
WN18RR	40,945	11	86,835
NELL-995	75,492	200	154,213
FB15k-237	14,505	237	310,116

Algorithm 1 Reasoning Algorithm CRule

Output: Query $(h, r, ?)$, initial KG KG_i
Input: Possible tail entities and their weights

function CATEGORIZATION(KG)
  Construct dict d, where $d[h][r]$ is a list of all entities that satisfy $(h, r, ?)$
  for h in entities **do**
    for r in relations **do**
      if $len(d[h][r]) > 1$ **then**
        Create new category node h_r ▷ category generation
  for (h, r, t) in KG **do**
    Replace e with category corresponding to e
    Replace t with h_r
    Add edge (h, r, h_r) to KG_c ▷ construct category-aware KG KG_c
  return KG_c

function GETRULES($KG_c, KG_i, data$)
  for $(h, r, t) \in data$ **do**
    $rules \leftarrow$ rules between h and t in KG_c based on Equation (1)
    if no $rules$ **then**
      $rules \leftarrow$ rules between h and t in KG_i based on Equation (1)
  return $rules$

function REASON($KG_i, data, rules$)
  for $(h, r, ?) \in data$ **do**
    for rule in $rules$ **do**
      $entities \leftarrow$ entities based on $rule$ and KG_i
      $weights \leftarrow$ Equation (2)
  return $tails$, $weights$

$KG_c \leftarrow$ CATEGORIZATION(KG_i)
$rules \leftarrow$ GETRULES($KG_c, KG_i, data_{train}$)
$tails$, $weights \leftarrow$ REASON($KG_i, data_{test}, rules$)

Baselines

We use four kinds of models as baselines, including AMIE and RuleN as symbolic models; DeepPath, MINERVA, and Multihop-KG as neural network-based multi-hop models; TransE, TransR, DistMult, ComplEx and ConvE as embedding-based models; MLN, Neural LP, and PRA as symbolic-machine learning combined models.

We do not report results of baselines for small datasets, as the results of CRule are close to 1.0. Due to generalization difficulty, symbolic methods' results have not been reported before. Hence, we do not employ them as baselines for large datasets.

Link Prediction

Link prediction is the most widely used evaluation task for multi-hop reasoning. For each query, we rank the candidate entities based on their weights in reverse order. All entities in the KGs are considered as candidate entities for all kinds of methods.

We use the following metrics: Mean Average Precision (MAP), Mean Reciprocal Rank (MRR) of correct entities, and the percentage of correct entities with ranks no larger than N (Hits@N). Higher values of these metrics indicate better model performance. The evaluation results are shown in Table 3 and 4.

Experiments verify that CRule exhibits near-perfect reasoning performance on small datasets. On larger datasets, it surpasses symbolic and embedding-based baselines, and achieves competitive results to classical neural network-based methods, even outperforms all baselines on WN18RR and FB15k-237.

The experiments show that although the categorization operation seems simple, it can preserve most semantic information in the original KG. Categorization enables the symbolic methods to be applicable to large-scale KGs, and even the most basic rule-based method can achieve competitive results based on categorized KG. Besides the good performance, CRule also has the advantages of training-free, non-parametric, explainable, etc.

CRule's performance is comparable to classical neural network methods but slightly inferior to state-of-the-art methods. To enhance reasoning

Table 3: Link prediction results (Hits@N & MRR) on all datasets. "ML" is short for "Machine Learning", "NN" is short for "Neural Network".

Dataset	Type	Model	Metric			
			Hits@1	Hits@3	Hits@10	MRR
Small Datasets						
Countries_S1	Symbolic (Ours)	CRule(s)/CRule	1.0	1.0	1.0	1.0
Countries_S2			0.917	1.0	1.0	0.958
Countries_S3			1.0	1.0	1.0	1.0
Grid-World	Symbolic (Ours)	CRule(s)/CRule	1.0	1.0	1.0	1.0
Large Datasets						
WN18RR	Embedding	TransE	0.182	0.382	0.497	0.223
		DistMult	0.410	0.441	0.475	0.433
		ComplEx	0.382	0.433	0.480	0.415
		ConvE	0.403	0.452	0.519	0.438
	Symbolic+ML	MLN	0.191	0.322	0.361	0.259
		Neural LP	0.376	0.468	0.657	0.463
	NN	MINERVA	0.413	0.456	0.513	0.448
		Multihop-KG	0.327	-	**0.564**	0.407
	Symbolic (Ours)	CRule(s)	**0.425**	**0.483**	0.545	**0.465**
		CRule	0.424	**0.483**	0.525	0.462
NELL-995	Embedding	TransE	0.241	0.392	0.413	0.307
		TransR	0.239	0.399	0.411	0.313
		DistMult	0.347	0.454	0.495	0.410
		ComplEx	0.382	0.473	0.522	0.467
		ConvE	0.452	0.564	0.629	0.587
	NN	MINERVA	**0.663**	**0.773**	0.831	0.725
		Multihop-KG	0.656	-	**0.844**	**0.727**
	Symbolic (Ours)	CRule(s)	0.586	0.682	0.715	0.637
		CRule	0.589	0.704	0.738	0.650
FB15k-237	Embedding	TransE	0.206	0.316	0.454	0.289
		TransR	0.229	0.331	0.513	0.291
		DistMult	0.193	0.307	0.409	0.243
		ComplEx	0.204	0.316	0.420	0.261
		ConvE	0.241	0.354	0.490	0.312
	Symbolic	AMIE	0.174	-	0.409	-
		RuleN	0.182	-	0.42	-
	Symbolic+ML	MLN	0.067	0.103	0.16	0.098
		Neural LP	0.166	0.248	0.348	0.227
	NN	MINERVA	0.217	0.329	0.456	0.293
		Multihop-KG	0.327	-	0.564	0.407
	Symbolic (Ours)	CRule(s)	0.354	0.500	0.620	0.447
		CRule	**0.358**	**0.505**	**0.630**	**0.451**

Table 4: Link prediction results (MAP) on different relations of datasets NELL-995 and FB15k-237. We report the results of 10 subtasks in detail as in previous work.

Dataset	Tasks	TransE	TransR	PRA	DeepPath	MINERVA	CRule(s)	CRule
NELL-995	athleteHomeStadium	0.718	0.722	0.859	0.846	**0.928**	0.868	0.869
	athletePlaysForTeam	0.627	0.673	0.547	0.721	**0.827**	0.696	0.700
	athletePlaysInLeague	0.773	0.912	0.841	0.927	0.952	0.949	**0.953**
	athletePlaysSport	0.876	0.963	0.474	0.917	**0.986**	0.924	0.930
	organizationHeadquarteredInCity	0.620	0.657	0.811	0.790	**0.945**	0.933	0.926
	organizationHiredPerson	0.719	0.737	0.599	0.790	0.830	0.847	**0.855**
	personBornInLocation	0.712	0.812	0.668	0.699	**0.827**	0.788	0.800
	personLeadsOrganization	0.751	0.772	0.700	0.755	0.830	0.840	**0.845**
	teamPlaysSport	0.761	0.814	0.791	0.696	0.875	0.842	**0.881**
	worksFor	0.677	0.692	0.681	0.711	**0.825**	0.785	0.774
	...							
	Overall	0.737	0.789	0.675	0.784	**0.884**	0.843	0.852
FB15k-237	teamSports	0.896	0.784	0.987	**0.955**	-	0.901	0.942
	birthPlace	0.403	0.417	0.441	**0.531**	-	0.457	0.457
	personNationality	0.641	0.720	**0.846**	0.823	-	0.831	0.832
	filmDirector	0.386	0.399	0.349	0.441	-	**0.519**	0.516
	filmWrittenBy	0.563	**0.605**	0.601	0.457	-	0.537	0.537
	filmLanguage	0.642	0.641	0.663	**0.670**	-	0.590	0.592
	tvLanguage	0.804	0.906	0.960	**0.969**	-	0.873	0.873
	captialOf	0.554	0.493	0.829	0.783	-	**0.957**	**0.957**
	organizationFounded	**0.390**	0.339	0.281	0.309	-	0.263	0.250
	musicianOrigin	0.361	0.379	0.426	**0.514**	-	0.455	0.455
	...							
	Overall	0.532	0.540	0.541	**0.572**	-	0.546	0.549

performance, hierarchical reinforcement learning can be employed on categorized KG, which we leave for future work.

Efficiency Analysis

The primary constraint on applying symbolic methods to large KGs is efficiency. We compare the efficiency of symbolic reasoning without categorization (referred to as “Rule”), CRule, and MINERVA by measuring the average running time for each task. Experiments are conducted on the same device, and results are shown in Table 6.

Experiments show that CRule not only breaks the complexity limitation symbolic methods faced when applied to large KGs, but also has high efficiency. “Rule” is much slower than CRule, its inefficiency makes it difficult to be employed in practice. RuleN also requires several hours to reason on FB15k-237 [4]. MINERVA is also much slower than CRule even ignored the time spent on optimal parameter searching. Furthermore, the simplified version of CRule, referred to as CRule(s), achieves higher efficiency while maintaining equivalent model performance.

To further investigate the cause of the efficiency gap, we analyze the KGs before and after categorization statistically, as illustrated in Table 5. We count the number of nodes and edges and calculate the global efficiency, which is the average efficiency of all pairs of nodes. The efficiency of a pair of nodes is the multiplicative inverse of the shortest path distance between them. For every edge in the original KG, an inverse edge was added, resulting in twice as many edges as the number of triples in Table 2. Table 5 shows that categorization may not necessarily reduce the size of KGs, in fact, it may even increase the number of nodes and edges significantly. This is because an entity may belong to multiple categories, leading to more nodes and edges being added to KGs. However, categorization can decrease the distance between nodes, thus improving the efficiency of rule extraction and enabling symbolic reasoning on large KGs.

Conclusions

This paper presents a simulation of the categorization process and proposes a category-aware symbolic multi-hop reasoning method that can extract rules from large KGs efficiently. Experiments show that CRule can not only match the

Table 5: Statistical analysis of KGs before and after categorization.

	NELL-995		FB15k-237	
	Original	Category-Aware	Original	Category-Aware
#Nodes	75,492	56,489	14,505	76,200
#Edges	308,426	752,105	620,232	6,086,720
Global Efficiency	0.104	0.118	0.375	0.417

Table 6: Average running time per task. "Rule" refers to CRule without categorization, i.e., extracting rules and reasoning on the original KG directly.

Dataset	MINERVA	Rule	CRule(s)	CRule
NELL-995	238.0s	>12h	**10.3s**	19.4s
FB15k-237	379.4s	>12h	**84.1s**	251.7s

reasoning performance of classical neural network models, but even outperform them in terms of efficiency. Furthermore, CRule also overcomes the complexity issue that symbolic reasoning approaches suffer when being applied to large KGs. This paper highlights the effectiveness of the categorization operation and its promising research potential.

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