TAR: Neural Logical Reasoning across TBox and ABox

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ABSTRACT
Many ontologies, i.e., Description Logic (DL) knowledge bases, have been developed to provide rich knowledge about various domains. An ontology consists of an ABox, i.e., assertion axioms between two entities or between a concept and an entity, and a TBox, i.e., terminology axioms between two concepts. Neural logical reasoning (NLR) is a fundamental task to explore such knowledge bases, which aims at answering multi-hop queries with logical operations based on distributed representations of queries and answers. While previous NLR methods can give specific entity-level answers, i.e., ABox answers, they are not able to provide descriptive concept-level answers, i.e., TBox answers, where each concept is a description of a set of entities. In other words, previous NLR methods only reason over the ABox of an ontology while ignoring the TBox. In particular, providing TBox answers enables inferring the explanations of each query with descriptive concepts, which make answers comprehensible to users and are of great usefulness in the field of applied ontology. In this work, we formulate the problem of neural logical reasoning across TBox and ABox (TA-NLR), solving which needs to address challenges in incorporating, representing, and operating on concepts. We propose an original solution named TAR for TA-NLR. Firstly, we incorporate description logic based ontological axioms to provide the source of concepts. Then, we represent concepts and queries as fuzzy sets, i.e., sets whose elements have degrees of membership, to bridge concepts and queries with entities. Moreover, we design operators involving concepts on top of fuzzy set representation of concepts and queries for optimization and inference. Extensive experimental results on two real-world datasets demonstrate the effectiveness of TAR for TA-NLR.

KEYWORDS
Neural logical reasoning, Knowledge representation learning.

1 INTRODUCTION
Along with the rapid development of high-quality large-scale knowledge infrastructures [2, 33], researchers are increasingly interested in exploiting knowledge bases for real-world applications, such as knowledge graph completion [7, 32] and entity alignment [34]. However, to take advantage of knowledge bases, a fundamental yet challenging task still remains unsolved, i.e., neural logical reasoning (NLR), which attempts to answer complex structured queries that include logical operations and multi-hop projections given the facts in knowledge bases with distributed representations [16]. Recently, efforts [16, 28, 29] have been made to develop NLR systems by designing strategies to learn geometric or uncertainty-aware distributed query representations, and proposing mechanisms to deal with various logical operations on these distributed representations.

However, existing neural logical reasoners cannot fully fulfill our needs. In many real-world scenarios, we not only expect entity-level answers, but also seek for more descriptive concept-level answers, where each of the concepts is a description of a set of entities. For example, as shown in Figure 1, the query asks “who will be interested in techniques that G. Hinton is investigating and Google is using?”. The answers are not only entity-level ABox answers as yellow circles: Meta, Amazon, MIT, and Y. LeCun, but also concept-level TBox answers as squares: AI Researchers, The Academia, and The Industry. In this example, the conceptual answer The Academia refers to a summary of a set consisting of Y. LeCun and MIT, and it is intuitively desirable for users and worth exploring. In biomedical applications, people may want to find the causes for a set of symptoms and expect both entity-level answers (such as SARS-CoV-2 causing Fever) as well as concept-level answers (such as Viral infections causing Fever). In this case, the answer constitutes a descriptive concept-level answer (e.g., Viral infections) that is a summary of a set of entity-level answers. Downstream tasks like online chatbots [25] and conversational recommender systems [37] also need to retrieve rich and comprehensive answers to provide better services. Thus, providing both entity-level and concept-level answers can highly improve their capability of generating more informative responses to users and enriching the semantic information in answers for downstream tasks.

Figure 1: An example of TA-NLR. The query is “who will be interested in techniques that G. Hinton is investigating and Google is using?”. The answers are not only entity-level ABox answers as yellow circles: Meta, Amazon, MIT, and Y. LeCun, but also concept-level TBox answers as squares: AI Researchers, The Academia, and The Industry.
From the perspective of ontologies, i.e., description logic (DL) based knowledge bases, the ability of providing both concept-level and entity-level answers corresponds to the capability of TA-NLR: neural logical reasoning across TBox, i.e., terminology axioms between two concepts, and ABox, i.e., assertion axioms between two entities or between a concept and an entity [4]. Previous NLR systems only support reasoning over ABox, while more general TA-NLR systems additionally support reasoning over the whole ontology which is highly useful in applied ontologies [12]. Therefore, the TA-NLR problem is more general than the regular NLR problem in terms of providing not only entity-level ABox answers, but also concept-level TBox answers. Note that such descriptive concepts are higher-level abstractions of the set of entities and are more informative than the set in some cases [11].

Therefore, from the perspective of users and downstream tasks, TA-NLR is helpful by jointly providing the more informative concept-level and entity-level answers. From the perspective of logic theory, TA-NLR is useful in ontological applications by jointly reasoning over TBox and ABox. However, existing methods [16, 28, 29] can hardly reach TA-NLR for the following reasons. On the one hand, concepts are excluded from the NLR systems. That is to say, previous NLR systems perform reasoning upon regular knowledge graphs where only entities and relations exist, which correspond to subsets of ABoxes. On the other hand, mechanisms for exploiting concepts have not been well established. Specifically, previous solutions only measure query-entity similarity for NLR, without considering concept representations and operators involving concepts, such as query–concept similarity.

Along this line, we propose an original solution named TAR for TA-NLR. TAR is a short name which stands for a TBox and ABox neural reasoner. The key challenges for addressing TA-NLR are the incorporation of concepts, representation of concepts, and operator on concepts. First, we observe that terminological axioms include taxonomic hierarchies of concepts, concept definitions, and concept subsumption relations [15]. To incorporate concepts into the TA-NLR system, we thus introduce some terminological axioms into the system to provide sources of concepts. Second, we find that fuzzy sets [21], i.e., sets whose elements have degrees of membership, can naturally bridge entities with concepts, i.e., vague sets of entities. Therefore, we represent concepts as fuzzy sets in TAR. Meanwhile, properly representing queries is the prerequisite of effectively operating on concepts. We find that fuzzy sets can also bridge entities with queries, i.e., vague sets of entity-level answers. The theoretically-supported, vague, and unparameterized fuzzy set predictor on triples (1p queries in Figure 2). FuzzQE [9], GNN-QE [38], and LogicE [26] directly represent entities and queries using embeddings with specially designed restrictions and interpreted them as fuzzy sets for NLR. However, these studies still focus on the regular NLR problem, while we are solving a more general problem that additionally gives concept-level TBox answers. Furthermore, we explicitly include concepts and represent them as fuzzy sets, whereas they represent only queries as fuzzy sets. Moreover, they either use fuzzy logic at the entity level, or use fuzzy sets with arbitrary numbers of elements as the tunable embedding dimension without reasonable interpretations. We interpret queries as fuzzy sets where each element represents the probability of an entity being an answer, aligning with the definition and the essence of fuzzy sets [21], i.e., sets where each element has a degree of membership. This allows us to fully exploit fuzzy logic and provides a theoretical foundation in fuzzy set theory.

We summarize the main contribution of this work as follows:

(1) To the best of our knowledge, we are the first to focus on the TA-NLR problem that aims at providing both entity-level ABox answers and concept-level TBox answers, which better satisfies the need of users, downstream tasks, and ontological applications;

(2) We propose an original solution TAR that properly incorporates, represents, and operates on concepts. We incorporate terminological axioms to provide sources of concepts and employ fuzzy sets as the representations of concepts and queries. Logical operations are supported by the well-established fuzzy set theory and operators involving concepts are rationally designed upon fuzzy sets;

(3) We conduct extensive experiments and demonstrate the effectiveness of TAR for TA-NLR. We publish in public two pre-processed benchmark datasets for TA-NLR and the implementation of TAR1 to foster further research.

2 RELATED WORK

2.1 Neural Logical Reasoning

Given the vital role of neural logical reasoning (NLR) in knowledge discovery and artificial intelligence, great efforts have been made to develop NLR systems recently. QQE [16] is the pioneering work in this field, the authors formulate the NLR problem and propose to simply use points in the embeddings space to represent logical queries. Q2B [28] claimed that the representation of each query in the embedding space should be a geometric region instead of a single point because each query is equivalent to a set of entity-level answers in the embedding space. Therefore, they use hyper-rectangles that can include multiple points in the embedding space to represent queries. HypE [10], ConE [36], and BetaE [29] extended Q2B by using more sophisticated geometric shapes or Beta distributions for query representation. However, these reasoners could only give extensional entity-level answers, while we focus on the more general TA-NLR problem that aims at additionally providing descriptive concepts. We bring neural logical reasoners to the stage of reasoning across TBox and ABox.

2.2 Fuzzy Logic for NLR

Besides representing logical queries as points, geometric regions, or distributions, more recent methods explore fuzzy logic [21] for NLR. CQD [1] used t-norm and t-conorms from the fuzzy logic theory to achieve high performance on zero-shot settings. More specifically, mechanisms are proposed for the inference stage on various types of queries, while only training the simple neural link predictor on triples (1p queries in Figure 2). FuzzQE [9], GNN-QE [38], and LogicE [26] directly represent entities and queries using embeddings with specially designed restrictions and interpreted them as fuzzy sets for NLR. However, these studies still focus on the regular NLR problem, while we are solving a more general problem that additionally gives concept-level TBox answers. Furthermore, we explicitly include concepts and represent them as fuzzy sets, whereas they represent only queries as fuzzy sets. Moreover, they either just use fuzzy logic at the entity level, or use fuzzy sets with arbitrary numbers of elements as the tunable embedding dimension without reasonable interpretations. We interpret queries as fuzzy sets where each element represents the probability of an entity being an answer, aligning with the definition and the essence of fuzzy sets [21], i.e., sets where each element has a degree of membership. This allows us to fully exploit fuzzy logic and provides a theoretical foundation in fuzzy set theory.

1https://anonymous.4open.science/r/TAR-5D7D
2.3 Ontology Representation Learning

Several methods have been developed to exploit ontologies from the perspective of distributed representation learning [23]. ELEM [22] and EmEL [27] learn geometric embeddings for concepts in ontologies. The key idea of learning geometric embeddings is that the embedding function projects the symbols used to formalize $EL^+\!$ axioms into an interpretation $I$ of these symbols such that $I$ is a model of the $EL^+\!$ ontology. Other approaches [8, 31] rely on regular graph embeddings or word embeddings and apply them to ontology axioms. Another line of research [17, 18] focuses on jointly incorporating concepts and roles (relations), and logical operators; we limit TAR to axioms within a TBox.

Our work is related to ontology representation learning in that we incorporate some description logic based ontological axioms in Section 3.1.2 to provide sources of concepts, and we exploit concepts with distributed representation learning in our proposed TAR for TA-NLR. Methods for representation learning with ontologies have previously only been used to answer link prediction tasks such as predicting protein–protein interactions or performing knowledge graph completion, which can be viewed as answering $lp$ queries in Figure 2 whereas we also focus on more complex queries as well as providing concept-level TBox answers.

3 METHODOLOGY

Incorporating, representing, and operating on concepts are the key components for a neural logical reasoner across ABox and TBox. In this section, we first formulate the TA-NLR problem along with the process of incorporating concepts into the reasoning system. Then we propose an original solution TAR for TA-NLR by designing concept representations and operators involving concepts. We introduce optimization and inference procedures in the end.

3.1 Incorporating Concepts

3.1.1 Regular NLR. The regular NLR problem is defined on knowledge graphs. A knowledge graph is formulated as $\mathcal{KG} = \{(h, r, t)\} \subseteq \mathcal{E} \times \mathcal{R} \times \mathcal{E}$, where $h$, $r$, and $t$ denote the head entity, relation, and tail entity in triple $(h, r, t)$, respectively. $\mathcal{E}$ and $\mathcal{R}$ refer to the entity set and the relation set in $\mathcal{KG}$.

In the context of NLR, as shown in Figure 2.(a), each triple $(h, r, t)$ is regarded as a positive sample of the $lp$ query $\exists \! ? : [h \overset{1}{\rightarrow} t]$ with an answer $t$ that satisfies $[h \overset{1}{\rightarrow} t](t)$, where $h$ is the anchor entity and $\overset{1}{\rightarrow}$ is the projection operation with relation $r$. Furthermore, the regular NLR problem may also address the intersection, union, and negation operations $\land$, $\lor$, and $\neg$ within queries. Thus, infinite types of queries can be found with the combinations of these logical operations. We consider the representative types of queries, which are listed and demonstrated with their graphical structures in Figure 2. For example, queries of type $pi$ in Figure 2.(c) are to ask $\exists \! ? : \{ (h_1 \overset{1}{\rightarrow} e_1) \land (h_2 \overset{2}{\rightarrow} e_2) \} (q)$.

Regular neural logical reasoners seek to provide entity-level answers for each query. In particular, the answers are a set of entities that satisfy the query. We predict the possibility of each candidate entity $e \in \mathcal{E}$ satisfying a query $\exists \! ? : [q](e)$. We then rank the $|\mathcal{E}|$ possibilities and select the top-$k$ entities in $\mathcal{E}$ as the set of answers. Since all the candidate answers are entities, we can only retrieve entity-level answers from the regular NLR systems.

3.1.2 NLR across TBox and ABox. A joint TBox and ABox neural logical reasoner is upon a description logic based knowledge base $\mathcal{KB}$, i.e., ontology, which is an ordered pair $(\mathcal{T}, \mathcal{A})$ for TBox $\mathcal{T}$ and ABox $\mathcal{A}$, where $\mathcal{T}$ is a finite set of terminological axioms and $\mathcal{A}$ is a finite set of assertion axioms. Specifically, terminological axioms within a TBox $\mathcal{T}$ are of the form $c_1 \sqsubseteq c_2$ where the symbol $\sqsubseteq$ denotes subsumption ($\text{subClassOf}$). In general, $c_1$ and $c_2$ can be concept descriptions that consist of concept names, quantifiers and roles (relations), and logical operators; we limit TAR to axioms where $c_1$ and $c_2$ are concept names that will not involve roles or logical operators [3]. In the followings, we do not distinguish between a concept name and a concept description unless there are special needs. Then, a TBox is:

$$\mathcal{T} \subseteq \{ c_1 \sqsubseteq c_j | c_i, c_j \in C \} \tag{1}$$

where $C$ denotes the set of concept names in $\mathcal{KB}$. $\mathcal{T}$ accounts for the source of concepts and the pairwise concept subsumption information in the TA-NLR system. Assertion axioms in $\mathcal{A}$ consist of two parts. One part is the role assertion that is expressed as:

$$\mathcal{A}_{ee} \subseteq \{ e_1, e_2 | e_1, e_2 \in \mathcal{E}, r \in \mathcal{R} \} \tag{2}$$

where $e_1, e_2 \in \mathcal{E}$ denote entities, $\mathcal{E}$ denotes the entity set in $\mathcal{KB}$, $r \in \mathcal{R}$ denotes the role assertion between $e_1$ and $e_2$, and $\mathcal{R}$ is the role set of $\mathcal{A}_{ee}$. $\mathcal{A}_{ee}$ accounts for the triple-wise relational information about entities and roles in TA-NLR. The other part within $\mathcal{A}$ is the concept instantiation between an entity $e \in \mathcal{E}$ and
a concept $c \in C$:

$$A_{cc} = \{ e \circ c \} \subseteq \mathcal{E} \times C,$$

(3)

where $e \circ c$ represents $e$ is an instance of $c$. $A_{cc}$ serves as the bridge between $T$ and $A_{cc}$ by providing pairwise links between entities and concepts.

Since we incorporate concepts in the TA-NLR systems, we are able to ask questions about concepts. In particular, for a query $\exists p: \{ q \}(?)$ of arbitrary type discussed in Section 3.1.1, we not only provide a set of entities of $\{ a_e \}$ as the entity-level ABox answers, but also infer an explanation for each query result by summarizing entity-level answers with descriptive concepts, yielding another set of concept-level answers $\{ a_c \}$ as the concept-level TBox answers. More specifically, as shown in Figure 2, the answers are no longer restricted to be $e \in \mathcal{E}$ (denoted by circles), they can also be $c \in C$ (denoted by squares). To achieve this goal, we predict the possibility of each candidate entity $e \in \mathcal{E}$ as well as the possibility of each candidate concept $c \in C$ satisfying a query $\exists p: \{ q \}(?)$. We then rank $|\mathcal{E}|$ predicted scores of candidate entities and $|C|$ predicted scores of candidate concepts. We select and combine the top-$k$ results from each set of candidates as the final answers of $q$ with entity-level and concept-level answers $\{ a \} = \{ a_e \} \cup \{ a_c \}$.

Note that the regular NLR problem is a sub-problem of the TA-NLR problem. First, regular NLR systems can only provide a subset of the answers provided by TA-NLR systems, i.e., $\{ a_e \} \subseteq \{ a \}$. Also, the entire $\mathcal{K}_G$ in the context of regular NLR is equivalent to $A_{cc}$ in the case of the TA-NLR problem, which is a subset of the ontology, i.e., $\mathcal{K}_G \subseteq \mathcal{K}_B$, leaving $T$ and $A_{cc}$ with conceptual information in the ontologies not explored. Therefore, the problem we investigate is more general in terms of providing more answers and reasoning over more complex knowledge bases.

### 3.2 Representing Concepts and Queries

In this subsection, we first introduce how to represent concepts as fuzzy sets in our proposed TAR for TA-NLR. Then we represent queries as fuzzy sets as well to prepare for the later operations that involve concepts and queries.

#### 3.2.1 Representing Concepts

We are motivated to represent concepts as fuzzy sets by the relationship between concepts and entities. We gain insights on such relationship from the basic definition of semantics in description logics [6]:

**Definition 1.** A terminological interpretation $I = (\mathcal{A}^I, I)$ over a signature $(C, E, R)$ consists of:

- a non-empty set $\mathcal{A}^I$ called the domain
- an interpretation function $I$ that maps:
  - every entity $e \in \mathcal{E}$ to an element $e^I \in \Delta^I$
  - every concept $c \in C$ to a subset of $\Delta^I$
  - every role (relation) $r \in \mathcal{R}$ to a subset of $\Delta^I \times \Delta^I$

As we use a function-free language [3], we set $\Delta^I$ to be the Herbrand universe [24] of our knowledge base, i.e., $\Delta^I = \mathcal{E}$. Therefore, according to Definition 1, the interpretation of concept $c^I$ is a subset of $\mathcal{E}$, which is finite. On the other hand, fuzzy sets [21] over the Herbrand Universe are finite sets whose elements have degrees of membership:

$$FS = \{ \mu(x_1), \mu(x_2), \ldots, \mu(x_{|FS|}) \},$$

(4)

where $\mu(\cdot)$ is the membership function that measures the degree of membership of each element. Therefore, we further interpret all concepts as fuzzy sets over the finite domain $\Delta^I = \mathcal{E} = \bar{E}^I$ for $c^I \in C^I$, where $\bar{E}^I$ and $C^I$ are the interpretation of the entity set and the concept set.

To obtain the degree of membership of entity $e_i$ in $c^I$, i.e., $\mu(e_i)$, we first randomly initialize the embedding matrix of concepts and entities $\mathcal{E}_e \in \mathbb{R}^{C \times d}$ and $\mathcal{E}_c \in \mathbb{R}^{E \times d}$ with Xavier uniform initialization [14], where $d$ is the embedding dimension. Then we obtain the embedding of each concept $c \in \bar{E}^I$ by looking up the rows of $\mathcal{E}_e$. The embedding then serves as the generator of the fuzzy set representation of each concept $FS_c$. Thus, we compute the similarities between each concept $c$ and every entity in our universe $e \in \mathcal{E} = \Delta^I$ as the degrees of membership of each entity in the fuzzy set:

$$FS_c = \{ \sigma(c \circ e^I) \} = c^I,$$

(6)

where symbol $\circ$ denotes matrix multiplication and $\cdot^I$ represents the matrix transposition. The measured similarities are then normalized to $(0, 1)$ using the hit-wise sigmoid function $\sigma(\cdot)$. Here, the set-wise operation to obtain $FS_c$ consists of $|\mathcal{E}|$ pair-wise operations on the entity-concept pairs; we use the same operator for Instantiation, which we will explain in Section 3.3.4.

#### 3.2.2 Representing Queries

Properly representing queries is the prerequisite of operating on concepts. Fuzzy sets are particularly suitable to represent not only concepts, but also queries, because interpretations of queries are essentially interpretations of concepts. More accurately, queries correspond to concept descriptions that may include concept names, roles (relations), quantifiers, and logical operations. We can use the same formalism designed for representing concepts to represent entities, i.e., as a special type of fuzzy set [30] that assigns the membership function $\mu(\cdot)$ to 1 for one exact entity and to 0 to all others. Consequently, we can interpret entities as concepts. As explained in Section 3.1.1, queries may consist of entities, relations, and logical operations. Therefore, queries are interpreted as concept descriptions and we regard entities within queries as singleton within concepts. Thus, we can use the
same description logic semantics [5] to interpret a query \( q \) and a concept \( c \) in Definition 1: an interpretation function \( I \) maps every query \( q \) to a subset of \( \Delta I \). As the Herbrand universe \( \Delta I = \mathcal{E} \) is finite, the interpretation of query \( q \) is fully determined by the fuzzy membership function

\[
q^I = (\mu(e_1), \mu(e_2), \ldots, \mu(e_n)).
\]

Besides, representing queries as fuzzy sets has other advantages. Firstly, fuzzy logic theory [21] well-equip us to interpret logical operations within queries as the vague and unparameterized fuzzy set operations. The preservation of vagueness is important in that TA-NLR requires uncertainty, rather than deductive reasoning that guarantees the correctness. Unparameterized operations are desirable because they require fewer data during training and are often more interpretable. Secondly, since concepts are already represented as fuzzy sets, it would be more convenient for us to employ the same form of representation and retain only one form of representation within the TA-NLR system. We explain how to represent queries as fuzzy sets in detail as the followings.

**Representing Atomic Queries.** Each multi-hop logical query consists of one or more Atomic Queries (AQ), where an AQ is defined as a query that only contains projection(s) \( \psi \) from an anchor entity without logical operations such as intersection \( \land \), union \( \lor \), and negation \( \neg \). Therefore, the first step to represent queries is to represent AQs. We obtain the embeddings of each entity \( e \in \mathbb{R}^d \) and the \( \ell \)th relation \( r \in \mathbb{R}^{d \times d} \) by looking up the rows of the randomly initialized entity embedding matrices \( E_e \in \mathbb{R}^{\left| \mathcal{E} \right| \times d} \) and \( E_r \in \mathbb{R}^{\left| \mathcal{R} \right| \times d} \) with Xavier uniform initialization [14]. Then, the generator for fuzzy set representation \( FS_{aq} \) of a valid AQ \( \{ e \xrightarrow{r_1} \ldots r_l \} \) is \( (e + r_1 + \ldots + r_l) \). Thus, we obtain the fuzzy set corresponding to the query \( aq \) as:

\[
FS_{aq} = \{ \sigma((e + r_1 + \ldots + r_l) \otimes E_r^e) \} = aq^I.
\]

Similar to the process of obtaining fuzzy set representations of concepts, Eq.\( 8 \) is to acquire the degrees of membership of every candidate \( e \in \mathcal{E} \) being an answer to a given AQ by computing their normalized similarities.

**Fusing Atomic Queries.** AQs are fused by logical operations to form multi-hop logical queries. Since AQs are already represented in fuzzy sets and we are equipped with the theoretically supported fuzzy set operations, we interpret logical operations as fuzzy set operations over concepts to fuse AQs into the final query representations.

For two fuzzy sets in domain \( \Delta I = \mathcal{E} \): \( FS_1 = \{ \mu_1(e_1), \ldots, \mu_1(e_n) \} \) and \( FS_2 = \{ \mu_2(e_1), \ldots, \mu_2(e_n) \} \), we have the intersection \( \land \) over the two fuzzy sets as:

\[
FS_\land = \{ \mu_\land(e_1), \ldots, \mu_\land(e_n) \} = FS_1 \land FS_2 = \{ \forall e \in \mathcal{E} : \mu_\land(e) = \land (\mu_1(e), \mu_2(e)) \}.
\]

and the union \( \lor \) over the two fuzzy sets as:

\[
FS_\lor = \{ \mu_\lor(e_1), \ldots, \mu_\lor(e_n) \} = FS_1 \lor FS_2 = \{ \forall e \in \mathcal{E} : \mu_\lor(e) = \lor (\mu_1(e), \mu_2(e)) \}
\]

and we have the negation \( \neg \) over \( FS \) as:

\[
FS_\neg = \{ \mu_\neg(e_1), \ldots, \mu_\neg(e_n) \} = \{ \forall e \in \mathcal{E} : \mu_\neg(e) = 1 - \mu(e) \}
\]

where a \( t \)-norm \( T : [0, 1] \times [0, 1] \mapsto [0, 1] \) is a generalisation of conjunction in logic [20]. Some examples of \( t \)-norms include the Gödel \( t \)-norm \( \min(x, y) = \min[x, y] \), the product \( t \)-norm \( T_{prod}(x, y) = x \cdot y \), and the Lukasiewicz \( t \)-norm \( T_{Luk}(x, y) = \max[0, x + y - 1] \) [35]. Analogously, a \( t \)-conorm \( \cup : [0, 1] \times [0, 1] \mapsto [0, 1] \) is dual to \( t \)-norm and generalises logical disjunction – given a \( t \)-norm \( T \), the complementary \( t \)-conorm is defined by \( \cup (x, y) = 1 - T(1 - x, 1 - y) \) [1]. The choice of the \( t \)-norm is a hyperparameter of TAR.

Thus, each query can be decomposed into AQs and represented as a fuzzy set with Eq.\( 8 \), and then fuzzy set representations of AQs are fused by the fuzzy set operations in Eq.\( 9 \), \( 10 \), and \( 11 \) to obtain the final representation of the query. Note that fuzzy set operations hold the property of closure, which means the input and output of these operations remain fuzzy sets. Thus, the final representation of each query is also a fuzzy set \( FS_\mathcal{Q} \).

**3.3 Operating on Concepts.**

In previous sections, we manage to prepare for designing operators involving concepts by representing concepts and queries in fuzzy sets. Here, we design operators involving concepts for concept retrieval, entity retrieval, subsumption, and instantiation.

3.3.1 Concept Retrieval. Concept retrieval is to provide concept-level TBox answers, i.e., \( \{ a_c \} \) as discussed in Section 3.1.2. We measure the possibility of each \( e \in C \) being an intensional concept-level answer of a given query upon fuzzy set representations. More specifically, we measure the similarity between \( FS_c \) and \( FS_q \) based on the Jensen-Shannon divergence \( D_{JS} \) [13], which is a symmetrized and smoothed version of the Kullback-Leibler divergence \( D_{KL} \). The similarity function \( S_{\mathcal{C}} \) is defined by:

\[
S_{\mathcal{C}} = -D_{JS}(P||Q) = -\frac{1}{2}D_{KL}(P||M) + \frac{1}{2}D_{KL}(Q||M)
\]

where \( M = \frac{1}{2} (P + Q) \), \( P \) and \( Q \) represent the normalized fuzzy set representations of the considered query and concept descriptions, which are given by:

\[
P = \frac{FS_c}{\max(\|FS_c\|_p, \epsilon)} \quad Q = \frac{FS_q}{\max(\|FS_q\|_p, \epsilon)}
\]

where \( \epsilon \) is a small value to avoid division by zero and \( p \) is the exponent value in the norm formulation \( \| \cdot \|_p \). \( S_{\mathcal{C}} \) is then used for model training and concept-level inference in Section 3.4.
3.3.2 Entity Retrieval. Entity retrieval aims to provide entity-level ABox answers; for this purpose, only query–entity similarities \( S_{Ent} \) need to be measured without the necessity of designing new mechanisms. Therefore, we follow the pioneering work [16] on NLR to represent each query as an embedding \( q = f(q; \Omega) \) and measure query–entity similarity \( S_{Ent} \) as:

\[
S_{Ent} = y - \|q - e\|_1
\]

(14)

where \( y \) is the margin, \( f(\cdot) \) denotes the function to obtain query embedding \( q \), and \( \Omega \) denotes the parameters of \( f(\cdot) \). We explain \( f(\cdot) \) in detail in supplementary materials.\(^3\)

3.3.3 Subsumption. As defined by Eq.(1), \( T \) supplies for relational information among concepts with the form of concept subsumptions. Although concepts are represented in fuzzy sets and we already designed mechanism to measure the similarity between two fuzzy sets, we can not directly apply the method in Section 3.3.1 for concept subsumptions. It is because we need to measure the degree of inclusion of one concept to another instead of the similarities between them. The degree of inclusion is asymmetrical and more complex than the similarity measurement. Therefore, we employ a neural network \( h(\cdot) \) to model the degree of inclusion:

\[
S_{Sub} = h(e_1 \oplus e_2; \theta)
\]

(15)

where symbol \( \oplus \) denotes matrix concatenation over the last dimension, and \( \theta \) denotes the parameters of \( h(\cdot) \). In this paper, \( h(\cdot) \) is a two-layer feed-forward network with ReLU activation. Note that we directly use the embeddings of concepts without interpreting concept in the Herbrand universe of entities \( \Lambda^E = E \) because neither concept-entity relationships need to be modeled nor logical operations need to be resolved.

3.3.4 Instantiation. As defined by Eq.(3), \( \mathcal{A}_{cc} \) bridges \( T \) and \( \mathcal{A}_{cc} \) by providing links between entities and concepts. Such links instantiate concept with its describing entities and thus offer relational information with the form of concept instantiation. Recall that in Section 3.2.1, we obtain the fuzzy set representation of concepts by computing the similarities between the given \( c \) and every candidate \( e \in \mathcal{E} \) with Eq.(6). In the case of concept instantiation, the set-wise computation Eq.(6) is degraded to pair-wise similarity measurement for each concept-entity pair:

\[
S_{Ins} = \sigma(c \oplus e^T)
\]

(16)

where \( c \in \mathbb{R}^d \) and \( e \in \mathbb{R}^d \) are the categorical embeddings of concept \( c \) and entity \( e \), respectively.

3.4 Optimization

The parameters to optimize in our model TAR include the entity embedding matrix \( E_e \), the concept embedding matrix \( E_c \) for the basic representation of concepts that is out of domain \( \Lambda^T \), the relation embedding matrix \( E_r, \theta \) in Section 3.3.3, and \( \Omega \) in Section 3.3.2. In the training stage, we sample \( m \) negative samples for each positive instance of concept-level answering \( [q](e^+) \) by corrupting \( e^+ \) with randomly sampled \( e^-_i \in C \). Similarly, negative samples for entity-level answering \( [q](e^+) \) are obtained by corrupting \( e^+ \) in \( [q](e^+) \) with randomly sampled \( e^-_i \in \mathcal{E} \). For subsumption and instantiation, both sides of the concept-concept pairs and concept-entity pairs are randomly corrupted following the same procedure. The loss of TAR is defined as:

\[
L = \frac{1}{4m} \sum_{n \in N} \sum_{i=1}^m \log \sigma(S_n^+ - S_n^-)
\]

(17)

where \( N = \{\text{Con, Ent, Sub, Ins}\} \) denotes the set of the four included task discussed Section 3.3, \( S_n^+ \) (or \( S_n^- \)) denotes the predicted similarity or degree of inclusion of the positive (or negative) sample according to task \( n \). The overall optimization process of \( L \) is outlined in Algorithm 1 in supplementary materials.

In the inference stage, we predict \( S_{Con} \) (or \( S_{Ent} \)) for every candidate concept \( c \in \mathcal{C} \) (or entity \( e \in \mathcal{E} \)) regarding to query \( q \) and select the top-\( k \) results to be the concept-level TBox answers \( \{a_k\} \) (or entity-level ABox answers \( \{a_k\} \)) for query \( q \). Thus, we are able to achieve TA-NLR by providing the comprehensive answers \( \{a\} = \{a_k\} \cup \{a_k\} \). Although subsumption in Section 3.3.3 and instantiation in Section 3.3.4 are not included in the inference stage, they empowered TAR to better represent and operate concepts by providing training instances and extra supervision signals.

4 EXPERIMENTS

We conduct extensive experiments to answer the following research questions: **RQ1** How to properly compare TAR with methods that do not give concept-level TBox answers? **RQ2** How does TAR perform for providing concept-level TBox answers? **RQ3** How does TAR perform for providing entity-level ABox answers? **RQ4** How do the introduced subsumption and instantiation operators affect the performance of TAR?

4.1 Experimental Settings

4.1.1 Baselines (RQ1). The considered baseline methods are the three most established methods in NLR, namely GQE [16], Q2B [28], and BetaE [29], along with a recent method FuzzQE [9] that applies fuzzy operations in a different way. Since the regular neural logical reasoners can only provide entity-level answers, we need to come up with a way to make them give concept-level answers, so as to be compared with our proposed TAR on concept-level reasoning.

Therefore, we introduce the One-more-hop experiment. That is, we exploit all the information given by \( KB = (T, A) \) and simply degrade concepts to entities in the training stage. Specifically, we first augment \( \mathcal{A}_{cc} \) by the transductive links provided by \( T \). Then we combine the augmented \( \mathcal{A}_{cc} \) and \( \mathcal{A}_{re} \) to form the new knowledge graph \( KG' \). Note that part of the entities in \( KG' \) are the degraded concepts and \( KG' \) contains an additional relation \( re \) to describe the isInstanceOf relationship between an entity and a concept. Thus, we construct training examples of various types of queries using \( KG' \) and update model parameters following [28].
Table 1: Con, Ent, Sub, Ins, and NLR correspond to statistics of the instances for Concept Retrieval, Entity Retrieval, Subsumption, Induction, and baseline NLR methods. For other query types in Figure 2, the statistics are the same for each of them.

|   | |E| |FS| |C| |R| |Partition | |Con-1p | |Con-other | |Ent-1p | |Ent-other | |Sub | |Ins | |NLR-1p | |NLR-other |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
|YAGO4 | 32,465 | 8,382 | 75 | |#Train | 189,338 | 10,000 | |101,417 | 10,000 | 16,644 | |83,291 | |184,708 | 10,000 |
|DBpedia | 28,824 | 981 | 327 | |#Train | 473,924 | 10,000 | |136,821 | 10,000 | 2,582 | |225,436 | |362,257 | 10,000 |

Table 2: Performance of providing concept-level TBox answers. The best results are in boldface.

|   | |1p | |3p | |2i | |3i | |MRR | |Hit@3 |
|---|---|---|---|---|---|---|---|---|---|---|
|YAGO4 | GQE [16] | 35.3 | 49.5 | 33.7 | 51.3 | 43.9 | 11.8 | 9.1 | 14.4 | 6.6 | 28.4 | 43.7 | 67.4 | 44.9 | 67.1 | 49.9 | 15.0 | 12.3 | 19.7 | 9.4 | 36.6 |
|   | Q2B [28] | 37.3 | 53.4 | 59.6 | 55.0 | 47.6 | 2.1 | 1.6 | 1.7 | 1.1 | 28.8 | 47.1 | 75.4 | 78.2 | 70.0 | 58.2 | 2.9 | 1.9 | 1.9 | 1.4 | 37.4 |
|   | BetaE [29] | 39.0 | 57.0 | 58.9 | 52.9 | 45.8 | 10.4 | 8.9 | 2.7 | 6.5 | 31.3 | 47.8 | 74.7 | 76.7 | 64.2 | 52.5 | 10.1 | 10.2 | 2.9 | 5.0 | 38.2 |
|   | FuzzQE [9] | 34.1 | 50.3 | 44.4 | 52.9 | 44.0 | 13.2 | 11.7 | 19.0 | 8.3 | 30.9 | 41.6 | 69.8 | 59.4 | 67.5 | 52.8 | 16.9 | 13.3 | 23.4 | 10.4 | 39.5 |
|   | TAR | 51.3 | 76.4 | 82.7 | 55.9 | 53.9 | 51.3 | 48.9 | 54.3 | 45.9 | 57.8 | 60.3 | 88.9 | 88.7 | 66.4 | 65.5 | 60.2 | 57.1 | 59.9 | 52.5 | 66.6 |
|DBpedia | GQE [16] | 27.1 | 35.5 | 32.5 | 30.5 | 32.0 | 14.0 | 14.7 | 9.8 | 11.8 | 23.1 | 28.7 | 42.9 | 40.0 | 32.5 | 36.0 | 13.0 | 14.4 | 7.2 | 10.7 | 25.0 |
|   | Q2B [28] | 26.4 | 35.7 | 32.6 | 30.4 | 32.9 | 13.5 | 14.4 | 10.3 | 11.2 | 22.7 | 28.2 | 41.4 | 38.0 | 32.7 | 33.5 | 11.7 | 13.0 | 8.4 | 9.3 | 24.0 |
|   | BetaE [29] | 20.4 | 38.7 | 40.0 | 32.9 | 34.2 | 14.8 | 11.4 | 5.6 | 9.0 | 24.1 | 34.1 | 45.4 | 50.8 | 37.2 | 41.2 | 14.6 | 10.9 | 4.9 | 8.0 | 27.4 |
|   | FuzzQE [9] | 26.7 | 34.7 | 32.1 | 28.1 | 28.4 | 16.9 | 16.5 | 13.1 | 14.6 | 23.5 | 29.0 | 39.2 | 38.2 | 30.5 | 29.7 | 15.6 | 15.9 | 11.2 | 12.7 | 24.7 |
|   | TAR | 55.0 | 80.8 | 80.7 | 42.9 | 36.7 | 42.0 | 28.5 | 63.4 | 64.9 | 55.0 | 62.4 | 83.7 | 83.6 | 50.9 | 43.7 | 45.0 | 29.9 | 67.2 | 67.3 | 59.3 |

In the inference stage, two sets of candidate entities are prepared for each query. The first is the regular entity-level candidate set, which can be ranked following the original papers [16, 28, 29]. Another set contains the degraded concepts. To predict the possibility of a concept being an answer of a query \( q'() \), we add one more projection operation with the relation \( r_{ec} \), so as to construct the query: \( [q']() = [q \stackrel{r_{ec}}{\leftarrow}]() \). In other words, concept-level reasoning is implicitly achieved by an additional hop asking the \textit{instanceOf} upon entity retrieval queries, i.e., the \\textit{One-more-hop}.

### 4.1.2 Datasets

We conduct experiments on two commonly-used real-world large-scale knowledge bases, namely YAGO4 and DBpedia. Specifically, we use English Wikipedia version\(^1\) of YAGO4 and 2016-10 release\(^4\) of DBpedia. To preprocess the dataset for the TA-NLR problem, we first filter out low-degree entities in \( A_e \) and \( A_{ee} \) with the threshold 5. Then we split \( A_{ee} \) to two sets with the ratio 95% and 5% for training and evaluation, respectively. We use the same procedure as BetaE [29] to construct instances of logical queries from \( A_{ee} = KG \). We use all the triples in \( A_{ee} \) in the training set as training examples of \( lp \) queries and randomly select certain amount of training and evaluation examples for each of the other types of queries as stated in Table 1. We then split the evaluation set of each type of queries to the validation set and the testing set. We summarize the statistics of datasets in Table 1.

### 4.1.3 Implementation Details

We implement TAR using PyTorch and conduct all the experiments with Nvidia RTX 3090 GPUs and Intel Xeon CPUs. In the training stage, the initial learning rate of the Adam [19] optimizer, the embedding dimension \( d \), and the batch size, are tuned by grid searching within \( \{1e^{-2}, 1e^{-3}, 1e^{-4}, 1e^{-5}\} \), \( \{128, 256, 512\} \), and \( \{256, 512, 1024\} \), respectively. We keep the number of corrupted negative samples for each positive sample \( m \), the small value \( e \), the exponent value \( p \), the margin \( y \), and the adopted type of \( l-norm \) as \( 4 \), \( 1^{-12} \), \( 1, 12 \), and \( T_{prod} \), respectively.

We employ early stop with validation interval of 50 and tolerance of 3 for model training. In the test phase, following [28], we use the filtered setting and report the averaged results of Mean Reciprocal Rank (MRR) and Hits@3 over 3 independent runs.

### 4.2 Concept-level TBox Answers (RQ2)

We conduct the \\textit{One-more-hop} experiment as described in Section 4.1.1 to answer RQ2. As shown in Table 2, our proposed TAR consistently outperforms baseline methods on various evaluation metric with large margins. For the basic queries summarized in Figure 2 that are simply projections and intersections, our proposed TAR significantly improved the performance of providing concept-level TBox answers, especially for the multiple projection queries \( lp \), \( 2p \), and \( 3p \). For extra queries in Figure 2 that are more complex in terms of including unions or combined logical operations, we even boosted the performance exponentially. The average performance of TAR is also significantly better than baseline methods.

The superior performance of TAR can be explained in two folds. First, due to the lack of reasoning capabilities across TBox and ABox, GQE, Q2B, and BetaE need to do reasoning over more complicated queries. For example, baseline methods need to do reasoning over an \( ip \) query \( \{(h_1 \stackrel{r_{ec}}{\rightarrow}) \land (h_2 \stackrel{r_{ec}}{\rightarrow})\}() \)\) to provide concept-level answers of an \( ip \) query \( \{(h_1 \stackrel{r_{ec}}{\rightarrow}) \land (h_2 \stackrel{r_{ec}}{\rightarrow})\}() \). Therefore, \( ip \) queries become \( 2p \) queries for baseline methods, \( 2p \) becomes \( 3p \), and so on. Thus, the complexity of the transformed queries limits the baseline performance. Second, explicit supervision signals for concept-level reasoning are not provided by the baselines. That is to say, since the concepts are degraded as entities, regular NLR methods could not explicitly feed the empirical error on concept-level answers back to update the model parameters. It is thus understandable that the baseline methods cannot perform well to provide

\(^1\)https://yago-knowledge.org/downloads/yago-4
\(^4\)http://downloads.dbpedia.org/wiki-archive/downloads-2016-10.html
The real-world places are in bold-face. As 6 out of the top 10 entities are correct (real places), we believe fuzzy sets are capable of representing concepts in domain $\Delta^c$ as vague sets of entities. Regarding the other 4 entities, we observe that they are representative sport teams, leagues, or companies of a corresponding region. Although they are not real places, it makes sense that they have high degrees of membership $\mu(\cdot)$ to $c$, as they are strongly associated to the corresponding places. Therefore, the results demonstrate that the fuzzy set based TAR is capable of taking the advantage of vagueness to explore the highly related entities.

### 4.5 Case Study of Concept Representation

To gain insights of the fuzzy set representation of concept learned in TAR, we present a case study on the concept "place" $c = \langle http://dbpedia.org/ontology/Place\rangle$. The entities of real-world places are highlighted in boldface. As 6 out of the top 10 entities are correct (real places), we believe fuzzy sets are capable of representing concepts in domain $\Delta^c$ as vague sets of entities. Regarding the other 4 entities, we observe that they are representative sport teams, leagues, or companies of a corresponding region. Although they are not real places, it makes sense that they have high degrees of membership $\mu(\cdot)$ to $c$, as they are strongly associated to the corresponding places. Therefore, the results demonstrate that the fuzzy set based TAR is capable of taking the advantage of vagueness to explore the highly related entities.

### 5 CONCLUSION

In conclusion, we formulated the TA-NLR problem that performs neural logical reasoning across TBox and ABox. This is a novel problem and of great importance for users, downstream tasks, and ontological applications. The key challenges for addressing TA-NLR are the incorporation of concepts, representation of concepts, and operator on concepts. Accordingly, we propose TAR that properly incorporates ontological axioms, represents concepts and queries as fuzzy sets, and operates on concepts based on fuzzy sets. Extensive experimental results demonstrate the effectiveness of TAR for TA-NLR. The processed datasets and code are ready to be published to foster further research of TA-NLR.
### A SUPPLEMENTARY MATERIALS

#### Details of Entity Retrieval

Here, we elaborate the method to obtain the query embedding $q$ for providing entity-level ABox answers, i.e., $f(\cdot)$ with parameters $\Omega$. We use the integrated implementation\(^1\) to obtain $q$. Specifically, the projection operation $x \mapsto \theta$ that projects an entity or query embedding $x$ with relation $\theta$ is resolved by:

$$q = x \oplus r,$$

where $x \in \mathbb{R}^d$ is another query embedding that is obtained in advance or an entity embedding obtained by looking up $E_e \in \mathbb{R}^{|E| \times d}$ by rows. The intersection of two query embeddings $q_1$ and $q_2$ is resolved by:

$$q = a(q_1 \oplus q_2; \Omega_1) * q_1 + a(q_1 \oplus q_2; \Omega_2) * q_2,$$

where $\oplus$ denotes matrix concatenation over the last dimension, $\Omega$ denotes the parameters of $a(\cdot)$, and $a(\cdot)$ is a two-layer feed-forward network with $\text{Relu}$ activation. $a(\cdot)_1$ and $a(\cdot)_2$ represent the first and second $d$ attention weights, respectively. The union of two query embeddings $q_1$ and $q_2$ is resolved by:

$$q = \max(q_1, q_2) - 1,$$

where $\max(\cdot, -1)$ denotes the max operation over the last dimension.

#### Additional Experiments

Table 1: Ablation Study on Subsumptions and Instantiation upon DBpedia dataset. The best Hit@3 results are in boldface.

| Subsumptions | 1p | 2p | 3p | 2i | 3i | pi | ip | 2u | up | avg |
|--------------|----|----|----|----|----|----|----|----|----|----|
| w/o CC       | 61.4 | 73.8 | 71.8 | 22.9 | 20.1 | 28.8 | 21.6 | 67.5 | 62.6 | 47.8 |
| w/o EC       | 58.9 | 69.7 | 68.0 | 42.8 | 39.6 | 41.2 | 22.0 | 66.4 | 62.9 | 52.4 |
| TAR          | 62.4 | 83.7 | 83.6 | 50.9 | 43.7 | 45.0 | 29.9 | 67.2 | 67.3 | 59.3 |

| Instantiation | 1p | 2p | 3p | 2i | 3i | pi | ip | 2u | up | avg |
|---------------|----|----|----|----|----|----|----|----|----|----|
| w/o CC        | 20.5 | 22.8 | 23.0 | 18.8 | 20.6 | 14.7 | 25.6 | 10.4 | 18.4 | 19.4 |
| w/o EC        | 19.4 | 19.1 | 20.5 | 19.1 | 20.1 | 15.0 | 25.7 | 9.1 | 20.3 | 18.7 |
| TAR           | 34.6 | 28.0 | 29.0 | 44.6 | 54.8 | 21.4 | 40.6 | 17.8 | 23.0 | 32.6 |

#### Algorithm 1 The learning procedure of TAR.

**Require**: An ontological knowledge base $\mathcal{KB} = (T, \{A_{ee}, A_{ec}\})$.

$\mathcal{E}$ denotes the set of entities;

$\mathcal{C}$ denotes the set of concept (names);

$\mathcal{R}$ denotes the set of relations.

**Ensure**: $E_e$ denotes the entity embedding matrix;

$E_c$ denotes the concept embedding matrix;

$E_r$ denotes the relation embedding matrix;

$\Theta$ denotes the parameters of $h(\cdot)$;

$\Omega$ denotes the parameters of $f(\cdot)$.

1: // Start training;
2: Initialize $E_e, E_c, E_r, \Theta$ and $\Omega$;
3: for each training episode do
4: // Concept Retrieval.
5: for each query $[q](\cdot)$ do
6: Sample a concept-level answer $c^+ \in \mathcal{C}$ as a positive instance and $m$ non-answer concepts $\{c_1^+, \cdots, c_m^+\}$ as negative instances;
7: Represent $c^+$ as $FS_c^+$ by Eq.(6);
8: Represent $q$ as $FS_q$ by Eq.(8), (9), (10), and (11);
9: Calculate $S_{Con_i}$ by Eq.(12) and (13) given $FS_c^+$ and $FS_q$;
10: for each negative instance $c_j^+$ do
11: Represent $c_j^+$ as $FS_c$ by Eq.(6);
12: Calculate $S_{Con_i}$ by Eq.(12) and (13) given $FS_c^+$ and $FS_q$;
end for
13: // Entity Retrieval.
14: for each query $[q](\cdot)$ do
15: Sample an entity-level answer $e^+ \in \mathcal{E}$ as a positive instance and $m$ non-answer entities $\{e_1^+, \cdots, e_m^+\}$ as negative instances;
16: for each pair of concepts $(c_1, c_2)$ do
17: Sample $m$ concepts $\{c_1^+, \cdots, c_m^+\}$ as negative instances;
18: $c_1, c_2 \leftarrow$ Look up $E_c$ by rows;
19: Calculate $S_{Sub}^{c_1}$ by Eq.(15) given $c_1$ and $c_2$;
20: for each negative instance $c_j^+$ do
21: $c_j^+ \leftarrow$ Look up $E_c$ by rows;
22: Calculate $S_{Sub}^{c_j}$ by Eq.(15) given $(c_1, c_j^+)$ or $(c_2^+, c_2)$ with equal probability;
end for
23: end for
24: // Subsumption.
25: for each pair of concepts $(c_1, c_2)$ do
26: Sample $m$ concepts $\{c_1^+, \cdots, c_m^+\}$ as negative instances;
27: $c_1, c_2 \leftarrow$ Look up $E_c$ by rows;
28: Calculate $S_{Sub}^{c_1}$ by Eq.(15) given $c_1$ and $c_2$;
29: for each negative instance $c_j^+$ do
30: $c_j^+ \leftarrow$ Look up $E_c$ by rows;
31: Calculate $S_{Sub}^{c_j}$ by Eq.(15) given $(c_1, c_j^+)$ or $(c_2^+, c_2)$ with equal probability;
end for
32: end for
33: // Instantiation.
34: for each pair of concept and entity $(c, e)$ do
35: Sample $m$ negative concepts $\{c_1^+, \cdots, c_m^+\}$;
36: Sample $m$ negative entities $\{e_1^+, \cdots, e_m^+\}$;
37: $e \leftarrow$ Look up $E_e$ by rows;
38: $e \leftarrow$ Look up $E_e$ by rows;
39: Calculate $S_{Ins}^{c_1}$ by Eq.(16) given $c$ and $e$;
40: for each negative concept $c_j^+$ do
41: $c_j^+ \leftarrow$ Look up $E_c$ by rows;
42: Calculate $S_{Ins}^{c_j}$ by Eq.(16) given $(c_j^+, e)$;
end for
43: end for
44: for each negative entity $e_j^+$ do
45: $e_j^+ \leftarrow$ Look up $E_e$ by rows;
46: Calculate $S_{Ins}^{e_j}$ by Eq.(16) given $(c, e_j^+)$;
end for
47: end for
48: Calculate $\mathcal{L}$ by Eq.(17);
49: Update $E_c \leftarrow \partial \mathcal{L} / \partial E_c$; Update $E_e \leftarrow \partial \mathcal{L} / \partial E_e$; Update $E_r \leftarrow \partial \mathcal{L} / \partial E_r$; Update $\Theta \leftarrow \partial \mathcal{L} / \partial \Theta$; Update $\Omega \leftarrow \partial \mathcal{L} / \partial \Omega$;
50: end for
51: return updated $E_e, E_c, E_r, \Theta$ and $\Omega$.

---

\(^1\)https://github.com/snap-stanford/KGReasoning