Joint Abductive and Inductive Neural Logical Reasoning

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ABSTRACT

Neural logical reasoning (NLR) is a fundamental task in knowledge discovery and artificial intelligence. NLR aims at answering multi-hop queries with logical operations on structured knowledge bases based on distributed representations of queries and answers. While previous neural logical reasoners can give specific entity-level answers, i.e., perform inductive reasoning from the perspective of logic theory, they are not able to provide descriptive concept-level answers, i.e., perform abductive reasoning, where each concept is a summary of a set of entities. In particular, the abductive reasoning task attempts to infer the explanations of each query with descriptive concepts, which make answers comprehensible to users and is of great usefulness in the field of applied ontology. In this work, we formulate the problem of the joint abductive and inductive neural logical reasoning (AI-NLR), solving which needs to address challenges in incorporating, representing, and operating on concepts. We propose an original solution named ABIN for AI-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 ABIN for AI-NLR.

KEYWORDS

Neural logical reasoning, Knowledge representation learning, Fuzzy logic.

1 INTRODUCTION

Along with the rapid development of high-quality large-scale knowledge infrastructures [2, 30], researchers are increasingly interested in exploiting knowledge bases for real-world applications, such as knowledge graph completion [6] and entity alignment [31]. 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 [15]. Recently, efforts [15, 26, 27] 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 specific entity-level answers, but also seek for more descriptive concept-level answers, where each of the concepts is a summary of a set of entities. For example, as shown in Figure 1, the query asks “who will be interested in something that G. Hinton is investigating and Google is deploying?”. The answers are not only extensional entity-level answers represented by yellow circles: Meta, Amazon, MIT, and Y. LeCun, but also intensional concept-level answers represented in the squares: AI Researchers, The Academia, and The Industry.

Figure 1: An example of Abductive and Inductive Neural Logical Reasoning. The query is “who will be interested in something that G. Hinton is investigating and Google is deploying?”. The answers are not only extensional entity-level answers represented by yellow circles: Meta, Amazon, MIT, and Y. LeCun, but also intensional concept-level answers represented in the squares: AI Researchers, The Academia, and The Industry.
answers. Downstream tasks like online chatbots [24] and conversational recommender systems [34] 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.

Along this line, we propose an original solution named ABIN for AI-NLR. ABIN is a shortname which stands for an ABduction and INduction reasoner. The key challenges for addressing AI-NLR are the incorporation of concepts, representation of concepts, and operator on concepts. First, we observe that ontologies include taxonomic hierarchies of concepts, concept definitions, and concept subsumption relations [14]. To incorporate concepts into the AI-NLR system, we thus introduce some description logic based ontological axioms into the system to provide sources of concepts. Second, we find that fuzzy sets [20], 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 ABIN. 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 operations enable us to resolve logical operations within queries. Thus, the adoption of fuzzy sets is an ideal solution for concepts and queries representation in AI-NLR. Then operators involving concepts can also be designed based on fuzzy sets, including query-concept operators for abduction, entity-concept operators for instantiation, and concept-concept operator for subsumption. Attributed to the well designed operators, a joint abductive and inductive neural logical reasoner can be achieved.

We summarize the main contribution of this work as follows:

- To the best of our knowledge, we are the first to focus on the AI-NLR problem that aims at providing both entity-level and concept-level answers so as to jointly achieve inductive and abductive neural logical reasoning, which better satisfies the need of users, downstream tasks, and ontological applications;
- We propose an original solution ABIN that properly incorporates, represents, and operates on concepts. We incorporate ontologies 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;
- We conduct extensive experiments and demonstrate the effectiveness of ABIN for AI-NLR. We publish in public two pre-processed benchmark datasets for AI-NLR and the implementation of ABIN 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 sophisticated NLR systems in recent years. GQE [15] 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 [26] 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

1https://github.com/lilv98/ABIN
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hyper-rectangles that can include multiple points in the embedding space to represent queries. HypE [9] extended Q2B by using hyperboloids in a Poincaré ball for distributed query representation. However, these methods can only deal with projection, intersection, and union, without considering negation. More recently, BetaE [27] proposed to use Beta distributions over the embedding space to represent queries for NLR. The advantage of using distributions over points or geometric regions is that they can properly handle queries with negations and queries without answers. However, these reasoners could only give extensional entity-level answers, while we focus on the more general AI-NLR problem that aims at additionally providing descriptive concepts to summarize the entity-level answers. We bring neural logical reasoners to the stage of abductive and inductive reasoning.

2.2 Fuzzy Logic for NLR

Besides representing logical queries as points, geometric regions, or distributions, more recent methods explore fuzzy logic [20] 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 (lp queries in Figure 2). FuzzQE [8] directly represented entities and queries using embeddings with specially designed restrictions and interpreted them as fuzzy sets for NLR. However, this study still focuses on the regular NLR problem, while we are solving a more general problem that additionally includes neural abductive reasoning. Furthermore, we explicitly include concepts and represent them as fuzzy sets, whereas FuzzQE represents only the query as fuzzy set. Moreover, CQD only uses fuzzy logic at the entity level and FuzzQE uses 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 [20], 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 for our work.

2.3 Ontology Representation Learning

Recently, several methods that exploit ontologies from the perspective of distributed representation learning have been developed [22]. ELEm [21] and EmEL [25] 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 [7, 29] rely on regular graph embeddings or word embeddings and apply them to ontology axioms. Another line of research [16, 17] focuses on jointly embedding entities and relations in regular knowledge graphs, as well as concepts and roles (relations) in ontological axioms. 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 ABIN for AI-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 abductive concept-level answers.

3 METHODOLOGY

Incorporating, representing, and operating on concepts are the three key components for an abductive and inductive neural logical reasoner. In this section, we first formulate the AI-NLR problem along with the process of incorporating concepts into the reasoning system. Then we propose an original solution ABIN for AI-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 $\mathcal{KG} = \{(h, r, t) \subseteq \mathcal{E} \times \mathcal{R} \times \mathcal{E}, \text{where } h, r, t \text{ denote the head entity, relation, and tail entity in triple }(h, r, t), \text{respectively, } \mathcal{E} \text{ and } \mathcal{R} \text{ refer to the entity set and the relation set in } \mathcal{KG}.$

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 $\exists q : [h \xrightarrow{r} (t)]$ with an answer $t$ that satisfies $[h \xrightarrow{r} (t)]$, where $h$ is the anchor entity and $\xrightarrow{r}$ 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 $\exists q : [(h1 \xrightarrow{r1} (z1)) \land (h2 \xrightarrow{r2} (z2))]$.

Regular neural logical reasoners seek to provide extensional entity-level answers for each query. In particular, the answers are a set of entities that satisfies the query by inductive reasoning. Following the definition of inductive reasoning [33], the given knowledge graph $\mathcal{KG}$ might give us very good reason to accept...
that each element of the set is an answer of the query, but it does not ensure that. Therefore, we predict the possibility of each candidate entity \( e \in E \) satisfying a query \( \exists ? : [q](?) \). We then rank the \( |E| \) possibilities and select the top-\( k \) entities in \( E \) as the set of answers. Since all the candidate answers are entities, we can only retrieve extensional entity-level answers from the regular NLR systems.

3.1.2 **Abductive and Inductive NLR.** A joint abductive and inductive neural logical reasoner is upon ontological axioms provided in a knowledge base \( \mathcal{KB} \), which is an ordered pair \( (T, \mathcal{A}) \) for TBox \( T \) and ABox \( \mathcal{A} \), where \( T \) is a finite set of terminological axioms and \( \mathcal{A} \) is a finite set of assertion axioms. Specifically, terminological axioms within a TBox \( T \) are of the form \( \exists R.e_1.e_2 \) where the symbol \( \exists \) denotes subsumption (subClassOf). In general, \( e_1 \) and \( e_2 \) can be concept descriptions that consist of concept names, quantifiers and roles (relations), and logical operators; we limit \( \mathcal{A} \) to axioms where \( e_1 \) and \( e_2 \) 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:

\[
T \subseteq \{e_1 \subseteq e_2 | e_1, e_2 \in C\}
\]  

(1)

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

\[
\mathcal{A}_{ee} \subseteq \{(e_1, r, e_2) | e_1, e_2 \in E, r \in \mathcal{R}\}
\]  

(2)

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

\[
\mathcal{A}_{ec} = \{e \bowtie c \} \subseteq E \times C,
\]  

(3)

where \( e \bowtie c \) represents \( e \) is an instance of \( c \). \( \mathcal{A}_{ec} \) serves as the bridge between \( T \) and \( \mathcal{A}_{ee} \) by providing pairwise links between entities and concepts.

Since we incorporate concepts in the AI-NLR systems, we are able to ask questions about concepts. For a query \( \exists ? : [q](?) \) of arbitrary type discussed in Section 3.1.1, we not only perform inductive reasoning that returns a set of entities \( \{a_e\} \) as the extensional entity-level answers, but also we perform abductive reasoning that infers 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 intensional concept-level answers. More specifically, as shown in Figure 2, the answers are no longer restricted to be \( e \in E \) (represented as circles), they can also be \( c \in C \) (represented as squares). To achieve this goal, we predict the possibility of each candidate entity \( e \in E \) as well as the possibility of each candidate concept \( c \in C \) satisfying a query \( \exists ? : [q](?) \). We then rank \( |E| \) 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 extensional entity-level and intensional concept-level answers \( a = \{a_e\} \cup \{a_c\} \).

![Figure 4: Illustration of the interpretation of a concept \( c^I \).](image)

Note that the regular NLR problem is a sub-problem of the AI-NLR problem. On the one hand, regular NLR systems can only provide a subset of the answers provided by abductive and inductive neural logical reasoners, i.e., \( \{a_e\} \subseteq \{a\} \). On the other hand, the entire \( \mathcal{KG} \) in the context of regular NLR is equivalent to \( \mathcal{A}_{ee} \) in the case of the AI-NLR problem, which is a subset of the ontological knowledge base, i.e., \( \mathcal{KG} \subseteq \mathcal{KB} \), leaving \( T \) and \( \mathcal{A}_{ee} \) 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 ABIN for AI-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 [5]:

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

- a non-empty set \( \Delta^I \) called the domain
- an interpretation function \( \cdot^I \) that maps:
  - every entity \( e \in E \) 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 [23] of our knowledge base, i.e., \( \Delta^I = E \). Therefore, according to Definition 1, the interpretation of concept \( c^I \) is a subset of \( E \), which is finite. On the other hand, fuzzy sets [20] 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 \( \Delta^I = E = \{e_1, e_2, \ldots, e_{|E|}\} \) as the elements of fuzzy sets \( \{x_1, x_2, \ldots, x_{|FS|}\} \). Thus, we have:

\[
c^I = \{\mu(e_1), \mu(e_2), \ldots, \mu(e_{|E|})\},
\]  

(5)
As the Herbrand universe for our language is always finite, the interpretation of concept \(c^T\) is fully determined by the fuzzy membership function \(\mu(\cdot)\) that assigns a degree of membership to each entity \(e \in c^T \in \Delta^T = \mathcal{E} = c^T \) for \(c^T \in C^T\), where \(C^T\) and \(C^T\) are the interpretation of the entity (name) set and the concept (name) set.

To obtain the degree of membership of entity \(e_i\) in \(c^T\), i.e., \(\mu(e_i)\), we first randomly initialize the embedding matrix of concepts and entities as \(E_c \in \mathbb{R}^{\vert C^T \vert \times d}\) and \(E_e \in \mathbb{R}^{\vert \mathcal{E} \vert \times d}\) with Xavier uniform initialization [13], where \(d\) is the embedding dimension. Then we obtain the embedding of each concept \(c \in \mathbb{R}^d\) by looking up the rows of \(E_c\). The embedding then serves as the generator of the fuzzy set representation of each concept \(F_{Sc}\). Thus, we compute the similarities between each concept \(c\) and every entity in our universe \(e \in \mathcal{E} = \Delta^T\) as the degrees of membership of each entity in the fuzzy set:

\[
F_{Sc} = \{\sigma(c \otimes E_c^T) = c^T, \quad (6)
\]

where symbol \(\otimes\) denotes matrix multiplication and \(\sigma^T\) represents the matrix transposition. The measured similarities are then normalized to \((0, 1)\) using the bit-wise sigmoid function \(\sigma(\cdot)\).

Here, the set-wise operation to obtain \(F_{Sc}\) 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 sets [28] that assigns the membership function \(\mu(\cdot)\) to 1 for exactly one 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 concepts. Thus, we can use the same description logic semantics [4] to interpret a query \(q\) and concept \(c\) in Definition 1: an interpretation function \(\mathcal{I}\) maps every query \(q\) to a subset of \(\Delta^T\). As the Herbrand universe \(\Delta^T = \mathcal{E}\) is finite, the interpretation of query \(q^T\) is fully determined by the fuzzy membership function

\[
q^T = (\mu(e_1), \mu(e_2), \ldots, \mu(e_{|\mathcal{E}|})). \quad (7)
\]

Besides, representing queries as fuzzy sets have other advantages. Firstly, fuzzy logic theory [20] well-equipped us to interpret logical operations within queries as the vague and unparameterized fuzzy set operations. The preservation of vagueness is important in that we are performing inductive and abductive reasoning that 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

![Figure 5: Illustration of the process of representing concepts and queries for abductive reasoning.](image)

the AI-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) \(\rightarrow\) 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 \(l^{th}\) relation \(r \in \mathbb{R}^d\) by looking up the rows of the randomly initialized entity embedding matrices \(E_c \in \mathbb{R}^{\vert \mathcal{E} \vert \times d}\) and \(E_e \in \mathbb{R}^{\vert \mathbb{R} \vert \times d}\) with Xavier uniform initialization [13]. Then, the generator for fuzzy set representation \(F_{S_{aq}}\) of an valid AQ \([ e \rightarrow r_1, \ldots, r_n \rightarrow (?) ]\) is \((e + r_1 + \cdots + r_n)\). Thus, we obtain the fuzzy set corresponding to the query \(aq\) as:

\[
F_{S_{aq}} = \{\sigma((e + r_1 + \cdots + r_n) \otimes E_e^T) = aq^T, \quad (8)\]

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 AQSs 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 AQSs into the final query representations.

For two fuzzy sets in domain \(\Delta^T = \mathcal{E}\): \(F_{S_1} = \{\mu_1(e_1), \ldots, \mu_1(e_{|\mathcal{E}|})\}\) and \(F_{S_2} = \{\mu_2(e_1), \ldots, \mu_2(e_{|\mathcal{E}|})\}\), we have the intersection \(\land\) over the two fuzzy sets as:

\[
F_{S_1} \land F_{S_2} = \{\forall e \in \mathcal{E} : \mu_1(e) = \top(\mu_2(e), \mu_2(e))\}, \quad (9)
\]

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

\[
F_{S_1} \lor F_{S_2} = \{\forall e \in \mathcal{E} : \mu_1(e) = \bot(\mu_2(e), \mu_2(e))\}, \quad (10)
\]

and we have the negation \(\neg\) over \(F_{S}\) as:

\[
F_{S_1} \neg = \{\mu(e), \ldots, \mu(e)\} = \{\forall e \in \mathcal{E} : \mu(e) = 1 - \mu(e)\}, \quad (11)
\]

where a \(\top\)-norm \(\top : [0, 1] \times [0, 1] \mapsto [0, 1]\) is a generalization of conjunction in logic [19]. Some examples of \(\top\)-norms include the Gödel
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 abduction, induction, subsumption, and instantiation.

3.3.1 Abduction. Abductive reasoning is to give explanations for a set of observations; here, the answers to a query are the observations that we summarize by descriptive concepts, i.e., provide \( \{a_c\} \) as discussed in Section 3.1.2. We measure the possibility of each \( c \in C \) 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 \( D_{JS} \) [12], which is a symmetrized and smoothed version of the Kullback-Leibler divergence \( D_{KL} \). The similarity function we use for abductive inference \( S_{Abd} \) is defined by:

\[
S_{Abd} = -D_{JS}(P||Q) = -\frac{1}{2}D_{KL}(P||M) + \frac{1}{2}D_{KL}(Q||M) \tag{12}
\]

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:

\[
P = \frac{FS_c}{\max(|FS_c|, p, \epsilon)} \quad Q = \frac{FS_q}{\max(|FS_q|, p, \epsilon)} \tag{13}
\]

where \( \epsilon \) is a small value to avoid division by zero and \( p \) is the exponent value in the norm formulation \( || \cdot ||_p \). \( S_{Abd} \) are then used for model training and abductive inference in Section 3.4.3.

3.3.2 Induction. Inductive reasoning aims to provide extensional entity-level answers; for this purpose, only query–entity similarities \( S_{Ind} \) need to be measured without the necessity of designing new mechanisms. Therefore, we follow the pioneering work [15] on NLR and to represent each query as an embedding \( q = f(q; \Omega) \) and measure query–entity similarity \( S_{Ind} \) for inductive reasoning:

\[
S_{Ind} = \gamma - ||q - e||_1 \tag{14}
\]

where \( \gamma \) 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 Section A.1.

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:

\[
S_{Sub} = h(e_1 \oplus e_2; \theta) \tag{15}
\]

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 \( \Delta^f = \mathcal{E} \) 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), \( \mathcal{A}_{ec} \) 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:

\[
S_{Ins} = \sigma(c \otimes e^T) \tag{16}
\]

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 ABIN include the entity embedding matrix \( E_e \), the concept embedding matrix \( E_c \) for the basic representation of concepts that is out of domain \( \Delta^f \), the relation embedding matrix \( E_{r} \) in Section 3.3.3, and \( \Theta \) in Section A.1. In the training stage, we sample \( m \) negative samples for each positive instance of abductive reasoning \( [q]|(e^+) \) by corrupting \( e^+ \) with randomly sampled \( \epsilon_i^+ \in \mathcal{C} \). Similarly, negative samples for induction \( [q]|(e^-) \) are obtained by corrupting \( e^- \) in \( [q]|(e^-) \) with randomly sampled \( \epsilon_i^- \in \mathcal{E} \). 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 ABIN is defined as

\[
\mathcal{L} = -\frac{1}{4m} \sum_{n \in N} \sum_{i=1}^{m} \log \sigma(S_n^+ - S_n^-) \tag{17}
\]
Table 1: Abd, Ind, Sub, Ins, and NLR correspond to statistics of the instances for Abduction, Induction, Subsumption, Induction, and baseline NLR methods, respectively. For other query types in Figure 2, the statistics are the same for each of them.

|          | |E| | |F| | |C| | |R| | Partition | | Abd-1p | Abd-other | Ind-1p | Ind-other | Sub | Ins | NLR-1p | NLR-other |
|----------|-----------------|---------|---------|---------|---------|--------|--------|--------|---------|--------|---------|--------|---------|--------|--------|---------|---------|
| YAGO4    | 32,465          | 8,382   | 85      | 136,821 | 10,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  |
| Dbpedia  | 28,824          | 981     | 327     | 53      | 362,257 | 10,000 | 184,708| 10,000 | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  | 1,000  |

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

In the inference stage, we predict \( S_{\text{Abd}} \) (or \( S_{\text{Ind}} \)) for every candidate concept \( c \in C \) (or entity \( e \in E \)) regarding to query \( q \) and select the top-k results to be the intensional concept-level answers \( \{a_c\} \) (or extensional entity-level answers \( \{a_e\} \)) for query \( q \). Thus, we are able to achieve the transductive links provided by \( \mathcal{T} \) by the comprehensive answers \( \{a\} = \{a_c\} \cup \{a_e\} \). Although subsumption in Section 3.3.3 and instantiation in Section 3.3.4 are not included in the inference stage, they empowered ABIN to better represent and operate concepts by providing training instances and extra supervision signals.

4 EXPERIMENTS

In this section, we conduct extensive experiments to answer the following research questions:

**RQ1** How to properly compare ABIN with methods that do not support abduction?

**RQ2** How does ABIN perform for abductive reasoning?

**RQ3** How does ABIN perform for inductive reasoning?

**RQ4** How do the introduced subsumption and instantiation operators affect the performance of ABIN?

4.1 Experimental Settings

4.1.1 Baselines (RQ1). The considered baseline methods are the three most established methods in NLR, namely GQE [15], Q2B [26], and BetaE [27], which employ points, geometric regions, and distributions to represent queries, respectively. Since the regular neural logical reasoners can only provide extensional entity-level answers with inductive reasoning, we need to come up with a way to make them give concept-level answers without explicitly trained on abduction instances, so as to be compared with our proposed ABIN on abductive reasoning.

Therefore, we introduce the *One-more-hop* experiment to serve as baselines for the abduction task. That is, we exploit all the information given by \( K\mathcal{B} = (\mathcal{T}, \mathcal{A}) \) and simply degrade concepts to entities in the training stage. Specifically, we first augment \( \mathcal{A}_{ee} \) by the transductive links provided by \( \mathcal{T} \). Then we combine the augmented \( \mathcal{A}_{ee} \) and \( \mathcal{A}_{ec} \) to form the new knowledge graph \( \mathcal{K}'G \). Note that part of the entities in \( \mathcal{K}'G \) are the degraded concepts and \( \mathcal{K}'G \) contains an additional relation \( r_{ee} \) to describe the instanceOf relationship between an entity and a concept. Thus, we construct training examples of various types of queries using \( \mathcal{K}'G \) and update model parameters following [26].

In the inference stage, two sets of candidate entities are prepared for each query. One of them is the regular entity-level candidate set for inductive reasoning, which can be ranked following the original papers [15, 26, 27]. The other set contains the degraded concepts for abductive reasoning. To predict the possibility of a concept being and intensional answer of a query \( \{q\} \), we add one more projection operation with the relation \( r_{ee} \), so as to construct the abductive query: \( \{q\}'(\{q\}, \{a\}) \). In other words, abductive reasoning is implicitly achieved by an additional hop asking the instanceOf upon inductive queries, i.e., the *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 version3 of YAGO4 and 2016-10 release4 of DBpedia. To preprocess the dataset for the AI-NLR problem, we first filter out low-degree entities in \( \mathcal{A}_{ee} \) and \( \mathcal{A}_{ec} \) with the threshold 5. Then we split \( \mathcal{A}_{ee} \) to two sets with the ratio 95% and 5% for training and evaluation, respectively. We use the same procedure as BetaE [27] to construct instances of logical queries from \( \mathcal{A}_{ee} = \mathcal{K}G \). We use all the triples in \( \mathcal{A}_{ee} \) 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 the pre-processed datasets in Table 1, where Abd, Ind, Sub, Ins, and Base represent the instances for abduction, induction, subsumption, instantiation, and the NLR baselines, respectively. The processed datasets along with the code for pre-processing will be published in public to foster further research.

4.1.3 Implementation Details. We implement ABIN using PyTorch5 and conduct all the experiments on Linux server with GPUs (Nvidia RTX 3090) and CPU (Intel Xeon). In the training stage, the initial learning rate of the Adam [18] optimizer, the embedding dimension \( d \), and the batch size, are tuned by grid searching within \([1e^{-1}, 1e^{-3}, 1e^{-4}], [128, 256, 512], \) 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 \( t \)-norm as 4, \( 1e^{-12}, 1, 12, \) 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 [26], we use the filtered setting and report the averaged results of Mean Reciprocal Rank (MRR) and Hits@3 over 3 independent runs.

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3https://yago-knowledge.org/downloads/yago-4
4http://downloads.dbpedia.org/wiki-archive/downloads-2016-10.html
5https://pytorch.org/
4.2 Abductive Reasoning (RQ2)

We conduct the One-more-hop experiment as described in Section 4.1.1 to answer RQ2. As shown in Table 2, our proposed ABIN consistently outperforms baseline methods on various evaluation metrics with large margins. For the basic queries summarized in Figure 2 that are simply projections and intersections, our proposed ABIN significantly improved the performance of abductive reasoning, especially for the multiple projection queries 1p, 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 ABIN is also significantly better than baseline methods.

The superior performance of ABIN can be explained for two reasons. First, due to the lack of abductive reasoning capabilities, GQE, Q2B, and BetaE need to do reasoning over more complicated queries. For example, baseline methods need to do reasoning over an IPP query \( [(h_1 \rightarrow p_2) \land (h_2 \rightarrow p_2)] \rightarrow (\neg ?) \) to provide intensional concept-level answers of an IPP query \( [(h_1 \rightarrow p_2) \land (h_2 \rightarrow p_2)] \). Therefore, IPP 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 abductive reasoning are not provided by the baseline methods. ABIN is designed for AI-NLR, it is interesting to know the performance of ABIN on inductive reasoning only (for answering RQ3).

The results of inductive reasoning tasks in Table 3 show that ABIN consistently outperforms baseline methods on various metrics. The performance gain of ABIN is credited to its additional information of the relationships among queries, entities, and concepts, which are helpful for inductive reasoning.

The average performance of ABIN is also significantly better than baseline methods. ABIN is designed for AI-NLR, it is interesting to know the performance of ABIN on inductive reasoning only (for answering RQ3).

4.4 Ablation Study (RQ4)

We conduct ablation study on DBpedia dataset to answer RQ4. As shown in Table 4, when the Subsumption task is not included, i.e.,
ontological axioms in $T$ are not used and $S_{Sub}$ is not computed, ABIN w/o $Sub$ underperforms ABIN on all types of queries for both abductive and inductive reasoning. Such results clearly demonstrate the importance of the relational information between concepts to be used for AI-NLR, and the effectiveness of the designed operator in Section 3.3.3 for handling such information. On the other hand, ABIN consistently outperforms w/o Ins on all types of queries. This verifies that the relational information about $is\text{InstanceOf}$ in $\mathcal{A}_{ec}$ is vital for AI-NLR, and the pair-wise degraded fuzzy set generation process introduced in Section 3.3.4 is effective to tackle with $\text{Instantiation}$. More experimental results about abduction study are reported in Table 6 in supplementary materials.

4.5 Case Study of Concept Representation

To gain insights of the fuzzy set representation of concept learned in ABIN, we present a case study on the concept “place”, $c = \langle http://dbpedia.org/ontology/Place \rangle$. The 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 $\Delta^F$ as vague sets of entities. Regarding to 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 ABIN is capable of take the advantage of vagueness to explore the highly related entities.

5 CONCLUSION

In conclusion, we formulated the AI-MLR problem that jointly performs abductive and inductive neural logical reasoning. This is a novel problem and of great importance for users, downstream tasks, and ontological applications. The key challenges for addressing AI-NLR are the incorporation of concepts, representation of concepts, and operator on concepts. Accordingly, we propose ABIN 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 ABIN for AI-NLR. The processed datasets and code are ready to be published to foster further research of AI-MLR.

Table 5: Top 10 entities with highest degrees of membership in concept “place” $c = \langle http://dbpedia.org/ontology/Place \rangle$. The real-world places are in boldface.

| Entity $e$                           | Info                                      | $\mu(e)$ |
|-------------------------------------|-------------------------------------------|----------|
| Province_of_L'Aquila (A province of Italy) | A province of Italy                       | 1.0000   |
| Lietuvos_krepšinio_lyga (A sport league in Lithuania) | A sport league in Lithuania              | 0.9888   |
| Moghreb_Tétouan (A sport team in Morocco)     | A sport team in Morocco                   | 0.9888   |
| Quebec_Route_132 (A highway in Canada)       | A highway in Canada                       | 0.9986   |
| School_of_Visual_Arts (A college in New York) | A college in New York                     | 0.9968   |
| League_of_Ireland (A sport league in Ireland) | A sport league in Ireland                | 0.9777   |
| Pančevo (A city in Serbia)                 | A city in Serbia                          | 0.9762   |
| Kolar (A city in India)                   | A city in India                           | 0.9755   |
| Kemco (A company in Japan)                | A company in Japan                        | 0.9740   |
| Deyr_County (A county in Iran)             | A county in Iran                          | 0.9740   |

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A  SUPPLEMENTARY MATERIALS

A.1  Inductive Reasoning in ABIN

Here, we elaborate the method to obtain the query embedding \( q \) for inductive reasoning, i.e., \( f(\cdot) \) with parameters \( \Omega \). We use the integrated implementation\(^7\) of GQE [15] to obtain \( q \). Specifically, the projection operation \( x \mapsto \) that project an entity or query embedding \( x \) with relation \( r \) is resolved by:

\[
q = x + r,
\]

where \( x \in \mathbb{R}^d \) is another query embedding that is obtained in advance or an entity 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:

\[
q = a(q_1 \odot q_2; \Omega)_1 * q_1 + a(q_1 \odot q_2; \Omega)_2 * q_2,
\]

where \( \odot \) 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 Relu activation. \( a(\cdot)_1 \) and \( a(\cdot)_2 \) represent the first and second attention weights, respectively. The union of two query embeddings \( q_1 \) and \( q_2 \) is resolved by:

\[
q = \max(q_1, q_2) - 1.
\]

Table 6: Ablation Study on Subsumptions and Instantiation upon DBpedia dataset. The best Hit@3 results are in boldface.

| Ablation | 1p | 2p | 3p | 2i | 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 |
| w/o EC   | 58.9 | 69.7 | 68.0 | 42.8 | 39.6 | 41.2 | 22.0 | 66.4 | 62.9 |
| ABIN     | 62.4 | 83.7 | 83.6 | 50.9 | 43.7 | 50.0 | 29.9 | 67.2 | 67.3 |

Induction

| Ablation | 1p | 2p | 3p | 2i | 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 |
| w/o EC   | 19.4 | 19.1 | 20.5 | 19.1 | 20.1 | 15.0 | 25.7 | 9.1 | 20.3 |
| ABIN     | 54.6 | 28.0 | 29.0 | 44.6 | 54.8 | 21.4 | 40.6 | 17.8 | 23.0 |

Algorithm 1 The learning procedure of ABIN.

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

\( \mathcal{E} \) 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:  // ABDUCTION.
5: for each query \([g](?)\) do
6:  Sample a concept-level answer \( c^+ \in \mathcal{C} \) as a positive instance and \( m \) non-answer concepts \( \{c^1_1, \cdots, c^1_m\} \) 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 \( S^+_{abd} \) by Eq.(12) and (13) given \( FS_c^+ \) and \( FS_q \);
10: for each negative instance \( c_i^- \) do
11:  Represent \( c_i^- \) as \( FS_c^- \) by Eq.(6);
12:  Calculate \( S^-_{abd} \) by Eq.(12) and (13) given \( FS_c^- \) and \( FS_q \);
13: end for
14: // INDUCTION.
15: for each query \([g](?)\) do
16:  Sample an entity-level answer \( e^+ \in \mathcal{E} \) as a positive instance and \( m \) non-answer entities \( \{e^1_1, \cdots, e^1_m\} \) as negative instances;
17:  \( e^+ \leftarrow \) Look up \( E_e \) by rows;
18:  \( q \leftarrow f(q; \Omega) \);
19:  Calculate \( S^+_{ind} \) by Eq.(14) given \( e^+ \) and \( q \);
20: for each negative instance \( e_i^- \) do
21:  \( e_i^- \leftarrow \) Look up \( E_e \) by rows;
22:  Calculate \( S^-_{ind} \) by Eq.(14) given \( e_i^- \) and \( q \);
23: end for
24: end for
25: // SUBSUMPTION.
26: for each pair of concepts \( (c_1, c_2) \) do
27:  Sample \( m \) concepts \( \{c^1_1, \cdots, c^1_m\} \) as negative instances;
28:  \( c_1, c_2 \leftarrow \) Look up \( E_e \) by rows;
29:  Calculate \( S^+_{sub} \) by Eq.(15) given \( c_1 \) and \( c_2 \);
30: for each negative instance \( c_i^- \) do
31:  \( c_i^- \leftarrow \) Look up \( E_e \) by rows;
32:  Calculate \( S^-_{sub} \) by Eq.(15) given \( c_i^- \) or \( (c_i^-, c_2) \) with equal probability;
33: end for
34: end for
35: // INSTANTIATION.
36: for each pair of concept and entity \( (c, e) \) do
37:  Sample \( m \) negative concepts \( \{c^1_1, \cdots, c^1_m\} \);
38:  Sample \( m \) negative entities \( \{e^1_1, \cdots, e^1_m\} \);
39:  \( e \leftarrow \) Look up \( E_e \) by rows;
40:  \( e \leftarrow \) Look up \( E_e \) by rows;
41:  Calculate \( S^+_{ins} \) by Eq.(16) given \( c \) and \( e \);
42: for each negative concept \( c_i^- \) do
43:  \( c_i^- \leftarrow \) Look up \( E_e \) by rows;
44:  Calculate \( S^-_{ins} \) by Eq.(16) given \( (c_i^-, e) \);
45: end for
46: for each negative entity \( e_i^- \) do
47:  \( e_i^- \leftarrow \) Look up \( E_e \) by rows;
48:  Calculate \( S^-_{ins} \) by Eq.(16) given \( (c, e_i^-) \);
49: end for
50: end for
51: Calculate \( \mathcal{L} \) by Eq.(17);
52: Update \( E_e \leftarrow \delta \mathcal{L} / \delta E_e \); Update \( E_c \leftarrow \delta \mathcal{L} / \delta E_c \); Update \( E_r \leftarrow \delta \mathcal{L} / \delta E_r \); Update \( \Theta \leftarrow \delta \mathcal{L} / \delta \Theta \); Update \( \Omega \leftarrow \delta \mathcal{L} / \delta \Omega \);
53: end for
54: return updated \( E_e, E_c, E_r, \Theta \) and \( \Omega \).

\(^7\)https://github.com/snap-stanford/KGReasoning