

Fuzzy Logic based Logical Query Answering on Knowledge Graphs

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Abstract

Answering complex First-Order Logical (FOL) queries on large-scale incomplete knowledge graphs (KGs) is an important yet challenging task. Recent advances embed logical queries and KG entities in the same space and conduct query answering via dense similarity search. However, most logical operators designed in previous studies do not satisfy the axiomatic system of classical logic, limiting their performance. Moreover, these logical operators are parameterized thus require many complex FOL queries as training data, which are often arduous to collect or even inaccessible in most real-world KGs. We thus present **FuzzQE**, a fuzzy logic based logical query embedding framework for answering FOL queries over KGs. **FuzzQE** follows fuzzy logic to define logical operators in a principled and learning-free manner, where only entity and relation embeddings require learning. **FuzzQE** can further benefit from labeled complex logical queries for training. Extensive experiments on two benchmark datasets demonstrate that **FuzzQE** provides significantly better performance in answering FOL queries compared to state-of-the-art methods. In addition, **FuzzQE** trained with only KG link prediction can achieve comparable performance to those trained with extra complex query data.

1 Introduction

Knowledge graphs (KGs), such as Freebase (Bollacker et al. 2008), YAGO (Rebele et al. 2016), and NELL (Mitchell et al. 2018), provide structured representations of facts about real-world entities and relations. One of the fundamental tasks over KGs is to answer complex queries involving logical reasoning, e.g., answering First-Order Logical (FOL) queries with existential quantification (\exists), conjunction (\wedge), disjunction (\vee), and negation (\neg). For instance, the question “Who sang the songs that were written by John Lennon or Paul McCartney but never won a Grammy Award?” can be expressed as the FOL query shown in Fig 1.

This task is challenging due to the size and the incompleteness of KGs. FOL query answering has been studied as a graph query optimization problem in the database community (Hartig and Heese 2007; Zou et al. 2011; Schmidt, Meier, and Lausen 2010). These methods traverse the KG to retrieve answers for each sub-query and then merge the re-

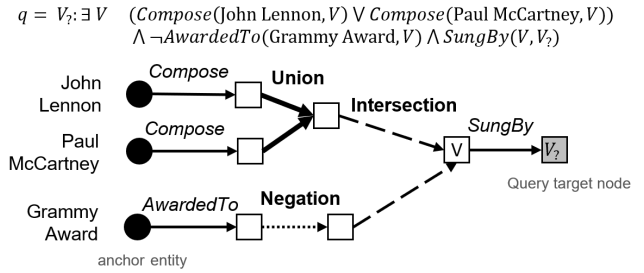


Figure 1: FOL query and its dependency graph for the question “Who sang the songs that were written by John Lennon or Paul McCartney but never won a Grammy Award?”.

sults. Though being extensively studied, these methods cannot well resolve the above-mentioned challenges. The time complexity of traversing on KG exponentially grows with the query complexity and is affected by the size of the intermediate results. This makes it difficult to scale to modern KGs, whose entities are often numbered in millions (Bollacker et al. 2008; Vrandečić and Krötzsch 2014). For example, Wikidata is one of the most influential KGs and reports that their query engine fails when the number of entities in a sub-query (e.g. people born in Germany) exceeds a certain threshold¹. In addition, real-world KGs are often incomplete, which prevents directly answering many queries by searching KGs. A recent study shows that only 0.5% of football players in Wikidata have a highly complete profile, while over 40% contain only basic information (Balaraman, Razniewski, and Nutt 2018).

To address the challenges of time complexity and KG incompleteness, a line of recent studies (Hamilton et al. 2018; Ren, Hu, and Leskovec 2020; Ren and Leskovec 2020) embed logical queries and entities into the same vector space. The idea is to represent a query using a *dependency graph* (Figure 1) and embed a complex logical query by iteratively computing embeddings from *anchor entities* to the *target node* in a bottom-up manner. The continuous and meaningful entity embeddings empower these approaches to handle missing edges. In addition, these models significantly reduce time and space complexity for inference, as they reduce

query answering to dense similarity matching of query and entity embeddings and can speed it up using methods like maximum inner product search (MIPS) (Shrivastava and Li 2014).

These methods nonetheless entail several limitations: First, the logic operators in these models are often defined ad-hoc, and many do not satisfy basic logic laws (e.g. the associative law $(\psi_1 \wedge \psi_2) \wedge \psi_3 \equiv \psi_1 \wedge (\psi_2 \wedge \psi_3)$ for logical formulae ψ_1, ψ_2, ψ_3), which limits their inference accuracy. Second, the logical operators of existing works are based on deep architectures, which require many training queries containing such logic operations to learn the parameters. This greatly limits the models’ scope of application, since it is challenging to collect a large number of reasonable complex queries with accurate answers.

Our goal is to create a logical query embedding framework that satisfies logical laws and provides learning-free logical operators. We hereby present **FuzzQE** (**Fuzzy Query Embedding**), a fuzzy logic based embedding framework for answering logical queries on KGs. We borrow the idea of fuzzy logic and use fuzzy conjunction, disjunction, and negation to implement logical operators in a more principled and learning-free manner. Our approach provides the following advantages over existing approaches: (i) **FuzzQE** employs differentiable logical operators that fully satisfy the axioms of logical operations and can preserve logical operation properties in vector space. This superiority is corroborated by extensive experiments on two benchmark datasets, which demonstrate that **FuzzQE** delivers a significantly better performance compared to state-of-the-art methods in answering FOL queries. (ii) Our logical operations do not require learning any operator-specific parameters. We conduct experiments to show that even when our model is only trained with link prediction, it achieves better results than state-of-the-art logical query embedding models trained with extra complex query data. This represents a huge advantage in real-world applications since complex FOL training queries are often arduous to collect. In addition, when complex training queries are available, the performance of **FuzzQE** can be further enhanced.

In addition to proposing this novel and effective framework, we propose some basic properties that an embedding model ought to possess as well as analyze whether existing models can fulfill these conditions. This analysis provides theoretical guidance for future research on embedding-based logical query answering models.

2 Related Work

Embedding entities in Knowledge Graphs (KGs) into continuous embeddings have been extensively studied (Bordes et al. 2013; Yang et al. 2015; Trouillon et al. 2016; Sun et al. 2019), which can answer one-hop relational queries via link prediction. These models, however, cannot handle queries with multi-hop (Guu, Miller, and Liang 2015) or complex logical reasoning. Hamilton et al. (2018) thus propose a graph-query embedding (GQE) framework that encodes a conjunctive query via a dependency graph with relation projection and conjunction (\wedge) as operators. Ren,

Hu, and Leskovec (2020) extend GQE by using box embedding to represent entity sets, where they define the disjunction (\vee) operator to support Existential Positive First-Order (EPFO) queries. Sun et al. (2020) concurrently propose to represent sets as count-min sketch (Cormode and Muthukrishnan 2005) that can support conjunction and disjunction operators. More recently, Ren and Leskovec (2020) further include the negation operator (\neg) by modeling the query and entity set as beta distributions. Friedman and Van den Broeck (2020) extend FOL query answering to probabilistic databases. These query embedding models have shown promising results to conduct multi-hop logical reasoning over incomplete KGs efficiently regarding time and space; however, we found that these models do not satisfy the axioms of either Boolean logic (Chvalovský 2012) or fuzzy logic (Klement, Mesiar, and Pap 2000), which limits their inference accuracy. To address this issue, our approach draws from fuzzy logic and uses the fuzzy conjunction, disjunction, and negation operations to define the logical operators in vector space.

In addition to the above logical query embedding models, a recent work CQD (Arakelyan et al. 2021) proposes training an embedding-based KG completion model (e.g. ComplEx (Trouillon et al. 2016)) to impute missing edges during inference and merge entity rankings with *t-norms* and *t-conorms* (Klement, Mesiar, and Pap 2000). Using beam search for inference, CQD has demonstrated strong capability of generalizing from KG edges to arbitrary EPFO queries. However, CQD has severe scalability issues since it involves scoring every entity for every atomic query. This is undesirable in real-world applications, since the number of entities in real-world KGs are often in millions (Bollacker et al. 2008; Vrandečić and Krötzsch 2014). Furthermore, its inference accuracy is thus bound by KG link prediction performance. In contrast, our model is highly scalable, and its performance can be further enhanced when additional complex queries are available for training.

3 Preliminaries

A knowledge graph (KG) consists of a set of triples $\langle e_s, r, e_o \rangle$, with $e_s, e_o \in \mathcal{E}$ (the set of entities) denoting the subject and object entities respectively and $r \in \mathcal{R}$ (the set of relations) denoting the relation between e_s and e_o . Without loss of generality, a KG can be represented as a First-Order Logic (FOL) Knowledge Base, where each triple $\langle e_s, r, e_o \rangle$ denotes an atomic formula $r(e_s, e_o)$, with $r \in \mathcal{R}$ denoting a binary predicate and $e_s, e_o \in \mathcal{E}$ as its arguments.

We aim to answer FOL queries expressed with existential quantification (\exists), conjunction (\wedge), disjunction (\vee), and negation (\neg).² The disjunctive normal form (DNF) of an FOL logical query q is defined as follows:

$$q[V?] \triangleq V? : \exists V_1, \dots, V_k (v_{11} \wedge \dots \wedge v_{1N_1}) \vee \dots \vee (v_{M1} \wedge \dots \wedge v_{MN_M})$$

²As in previous works (Ren, Hu, and Leskovec 2020; Arakelyan et al. 2021; Ren and Leskovec 2020), we do not consider FOL queries with universal quantification (\forall). Queries with universal quantification do not apply in real-world KGs since no entity connects with all the other entities.

Table 1: Here we list eight logic laws (I - VIII) from classical logic (Zimmermann 1991) and give the corresponding properties that a query embedding model should possess. ψ_1, ψ_2, ψ_3 represent logical formulae. ϕ denotes the scoring function that estimates the probability that the entity e can answer the query q . $\phi(q, e) \uparrow \Rightarrow \phi(\neg q, e) \downarrow$ means $\phi(\neg q, e)$ is monotonically decreasing with regard to $\phi(q, e)$. The full axiomatic systems and analysis are provided in Appendix C.

	Logic Law	Model Property
\wedge	I Conjunction Elimination $\psi_1 \wedge \psi_2 \rightarrow \psi_1$ $\psi_1 \wedge \psi_2 \rightarrow \psi_2$	$\phi(q_1 \wedge q_2, e) \leq \phi(q_1, e)$ $\phi(q_1 \wedge q_2, e) \leq \phi(q_2, e)$
	II Commutativity $\psi_1 \wedge \psi_2 \leftrightarrow \psi_2 \wedge \psi_1$	$\phi((q_1 \wedge q_2), e) = \phi((q_2 \wedge q_1), e)$
	III Associativity $(\psi_1 \wedge \psi_2) \wedge \psi_3 \leftrightarrow \psi_1 \wedge (\psi_2 \wedge \psi_3)$	$\phi((q_1 \wedge q_2) \wedge q_3, e) = \phi(q_1 \wedge (q_2 \wedge q_3), e)$
\vee	IV Disjunction Amplification $\psi_1 \rightarrow \psi_1 \vee \psi_2$ $\psi_2 \rightarrow \psi_1 \vee \psi_2$	$\phi(q_1, e) \leq \phi(q_1 \vee q_2, e)$ $\phi(q_2, e) \leq \phi(q_1 \vee q_2, e)$
	V Commutativity $\psi_1 \vee \psi_2 \leftrightarrow \psi_2 \vee \psi_1$	$\phi((q_1 \vee q_2), e) = \phi((q_2 \vee q_1), e)$
	VI Associativity $(\psi_1 \vee \psi_2) \vee \psi_3 \leftrightarrow \psi_1 \vee (\psi_2 \vee \psi_3)$	$\phi((q_1 \vee q_2) \vee q_3, e) = \phi(q_1 \vee (q_2 \vee q_3), e)$
	VII Involution $\neg \neg \psi_1 \rightarrow \psi_1$	$\phi(q, e) = \phi(\neg \neg q, e)$
\neg	VIII Non-Contradiction $\psi_1 \wedge \neg \psi_1 \rightarrow \bar{0}$	$\phi(q, e) \uparrow \Rightarrow \phi(\neg q, e) \downarrow$

where $V_?$ is the *target* variable of the query, and V_1, \dots, V_K denote the bound variable nodes. Each v_{mn} ($m = 1, \dots, M, n = 1, \dots, N_m$) represents a literal, i.e. a logical atom or the negation of a logical atom:

$$v_{mn} = \begin{cases} r(e, V) & r \in \mathcal{R}, e \in \mathcal{E}, V \in \{V_?, V_1, \dots, V_K\} \\ \neg r(e, V) & r \in \mathcal{R}, e \in \mathcal{E}, V \in \{V_?, V_1, \dots, V_K\} \\ r(V, V') & r \in \mathcal{R}, V, V' \in \{V_?, V_1, \dots, V_K\}, V \neq V' \\ \neg r(V, V') & r \in \mathcal{R}, V, V' \in \{V_?, V_1, \dots, V_K\}, V \neq V' \end{cases}$$

The goal of answering the logical query q is to find a set of entities $S_q = \{a | a \in \mathcal{E}, q[a] \text{ holds true}\}$, where $q[a]$ is a logical formula that substitutes the query target variable $V_?$ with the entity a .

A query can be considered as a combination of multiple sub-queries. For example, the query $q[V_?] = V_? : \text{Compose}(\text{John Lennon}, V_?) \wedge \text{Compose}(\text{Paul McCartney}, V_?)$ can be considered as $q_1 \wedge q_2$, where

$$q_1[V_?] = V_? : \text{Compose}(\text{John Lennon}, V_?) \\ q_2[V_?] = V_? : \text{Compose}(\text{Paul McCartney}, V_?)$$

Formally, we have:

$$S_{q_1 \wedge q_2} = S_{q_1} \cap S_{q_2}; \quad S_{q_1 \vee q_2} = S_{q_1} \cup S_{q_2}; \quad S_{\neg q} = S_q^c$$

where $(\cdot)^c$ denote set complement respectively.

Notation wise, we use boldfaced notations \mathbf{p}_e and \mathbf{S}_q to represent the embedding for entity e and the embedding for S_q , i.e. the answer entity set for query q , respectively. We use ψ_1, ψ_2, ψ_3 to denote logical formulae.

3.1 Logic Laws and Model Properties

The general idea of logical query embedding models is to recursively define the embedding of a query (e.g., $q_1 \wedge q_2$) based on logical operations on its sub-queries' embeddings (e.g., q_1 and q_2). These logical operations have to satisfy logic laws, which serve as additional constraints to learning-based query embedding models. Unfortunately, most existing query embedding models have (partially) neglected these laws, which result in inferior performance.

In this section, we study these logic laws shared by both classical logic and basic fuzzy logic (Zimmermann 1991) and deduce several basic properties that the logical operators should possess. The logic laws and corresponding model properties are summarized in Table 1.

Axiomatic systems of logic Let \mathcal{L} be the set of all the valid logic formulae under a logic system, and $\psi_1, \psi_2, \psi_3 \in \mathcal{L}$ represent logical formulae. $I(\cdot)$ denotes the truth value of a logical formula. The semantics of Boolean Logic are defined by (i) the interpretation $I : \mathcal{L} \rightarrow \{0, 1\}$, (ii) the Modus Ponens inference rule “from ψ_1 and $\psi_1 \rightarrow \psi_2$ infer ψ_2 ”, which characterizes logic implication (\rightarrow) as follows:

$$\psi_1 \rightarrow \psi_2 \quad \text{holds if and only if} \quad I(\psi_2) \geq I(\psi_1)$$

and (iii) a set of axioms written in Hilbert-style deductive systems (Klir and Yuan 1995). Those axioms define other logic connectives via logic implication (\rightarrow); for example, the following three axioms characterize the conjunction (\wedge) of Boolean logic (Chvalovský 2012):

$$\begin{aligned} \psi_1 \wedge \psi_2 &\rightarrow \psi_1 \\ \psi_1 \wedge \psi_2 &\rightarrow \psi_2 \\ (\psi_3 \rightarrow \psi_1) &\rightarrow ((\psi_3 \rightarrow \psi_2) \rightarrow (\psi_3 \rightarrow \psi_1 \wedge \psi_2)) \end{aligned}$$

The first two axioms guarantee that the truth value of $\psi_1 \wedge \psi_2$ never exceeds the truth values of ψ_1 and ψ_2 , and the last one enforces that $I(\psi_1 \wedge \psi_2) = 1$ if $I(\psi_1) = I(\psi_2) = 1$. The three axioms also imply commutativity and associativity of \wedge .

Model properties Let $\phi(q, e)$ be the embedding model scoring function estimating the probability that the entity e can answer the query q . This means that $\phi(q, e)$ estimates the truth value $I(q[e])$, where $q[e]$ is a logical formula that uses e to fill q . For example, given the query $q = V_? : \text{Compose}(\text{John Lennon}, V_?)$ and the entity $e = \text{“Let it Be”}$, $\phi(q, e)$ estimates the truth value of the logical formula $\text{Compose}(\text{John Lennon}, \text{Let it Be})$. We can thus use logic laws to deduce reasonable properties that a query embedding model should possess. For instance, $\psi_1 \wedge \psi_2 \rightarrow \psi_1$ is an axioms that characterizes logic conjunction (\wedge), which enforces that $I(\psi_1 \wedge \psi_2) \leq I(\psi_1)$, and we accordingly expect the embedding model to satisfy $\phi(q_1 \wedge q_2, e) \leq \phi(q_1, e)$, i.e., an entity e is less likely to satisfy $q_1 \wedge q_2$ than q_1 .

Table 2: Comparisons of different models regarding the properties of logical operations. *Expressivity* indicates whether the model can handle such logical operations, and *closed* indicates whether the embedding is in a closed form. *Commu.*, *Asso.*, *Elim.*, *Ampli.*, *Inv.* and *Non-contr.* stand for commutativity, associativity, conjunction elimination, disjunction amplification, involution, and non-contradiction respectively.

	\wedge				\vee				\neg		
	Expressivity (Closed)	Com.	Asso.	Elim.	Expressivity (Closed)	Com.	Asso.	Ampli.	Expressivity (Closed)	Inv.	Non-Contr.
GQE	$\checkmark(\checkmark)$	\checkmark	\times	\times	$\checkmark(\times)$	\checkmark	\checkmark	\checkmark	\times	N/A	N/A
Query2Box	$\checkmark(\checkmark)$	\checkmark	\checkmark	\checkmark	$\checkmark(\times)$	\checkmark	\checkmark	\checkmark	\times	N/A	N/A
BetaE	$\checkmark(\checkmark)$	\checkmark	\times	\times	(i) DNF $\checkmark(\times)$	\checkmark	\checkmark	\checkmark	$\checkmark(\checkmark)$	\checkmark	\times
					(ii) DM $\checkmark(\checkmark)$			\times			
FuzzQE	$\checkmark(\checkmark)$	\checkmark	\checkmark	\checkmark	$\checkmark(\checkmark)$	\checkmark	\checkmark	\checkmark	$\checkmark(\checkmark)$	\checkmark	\checkmark

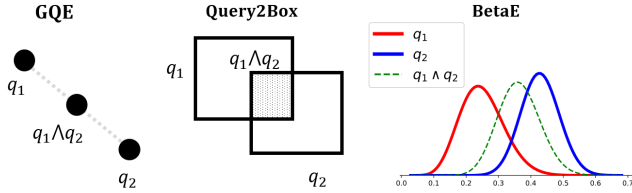


Figure 2: Illustration of query embeddings and embeddings of conjunctive queries in GQE, Query2Box, and BetaE. The conjunction operators takes embeddings of queries q_1, q_2 as input and produce an embedding for $q_1 \wedge q_2$.

Based on the axioms and deduced logic laws of classical logic (Fodor and Roubens 1994), we summarize a series of model properties that an embedding model should possess in Table 1. The list is not exhaustive but indicative.

3.2 Analysis of Prior Models on Model Properties

This section examines three representative logical query embedding models, namely GQE (Hamilton et al. 2018), Query2Box (Ren, Hu, and Leskovec 2020), and BetaE (Ren and Leskovec 2020), regarding their capability of satisfying the properties in Table 1. We summarize our findings in Table 2. GQE, Query2Box, BetaE represent queries as vectors, boxes (axis-aligned hyper-rectangles), and Beta distributions, respectively. The embedding-based logical operators transform embeddings of sub-queries into embeddings of the outcome query. The details about logical operator implementation of these models are given in Appendix D.

Conjunction (\wedge) Fig. 2 illustrates embedding-based conjunction operators of the three models, which takes embeddings of queries q_1, q_2 as input and produce an embedding for $q_1 \wedge q_2$. GQE, Query2Box, and BetaE are purposely constructed to be permutation invariant (Hamilton et al. 2018; Ren, Hu, and Leskovec 2020; Ren and Leskovec 2020), and their conjunction operators all satisfy *commutativity* (Law II). The conjunction operators of GQE and BetaE do not satisfy *associativity* (III) since they rely on the operation of averaging, which is not associative. GQE does not satisfy *conjunction elimination* (I); for example, supposing that $\mathbf{p}_e = \frac{1}{2}(\mathbf{S}_{q_1} + \mathbf{S}_{q_2})$ and $\mathbf{S}_{q_1} \neq \mathbf{S}_{q_2}$, we have $\phi(q_1 \wedge q_2, e) > \phi(q_1, e)$. BetaE does not satisfy *conjunction*

elimination (I) for similar reasons.

Disjunction (\vee) Previous works handle disjunction in two ways: the *Disjunctive Normal Form (DNF)* rewriting approach proposed by Query2Box (Ren, Hu, and Leskovec 2020), and the *De Morgan’s law (DM)* approach proposed by BetaE (Ren and Leskovec 2020). The DNF rewriting method involves rewriting each query as a DNF to ensure that the disjunction only appears in the last step, which enables the model to simply retain all input embeddings. The model correspondingly cannot represent the disjunction result as a closed form; for example, the disjunction of two boxes remains two separate boxes instead of one (Ren, Hu, and Leskovec 2020). The DM approach uses De Morgan’s law $\psi_2 \vee \psi_1 \equiv \neg(\neg\psi_2 \wedge \neg\psi_1)$ to compute the disjunctive query embedding, which requires the model to have a conjunction operator and a negation operator. This approach advantageously produces representation in a closed form, allowing disjunction to be performed at any step of the computation. The disadvantage is that if the negation operator does not work well, the error will be amplified and affect disjunction. The BetaE_{DM} does not satisfy *disjunction amplification* (IV) since its negation operator violates *non-contradiction* (VIII).

Negation To the best of our knowledge, BetaE is the only previous model that can handle negation. BetaE has proved that its negation operator is *involutory* (VII). However, this operator lacks the *non-contradiction* property (VIII), as for BetaE $\phi(\neg q, e)$ is not monotonically decreasing with regard to $\phi(q, e)$. An illustration is given in Appendix D.2.

3.3 Fuzzy Logic

Fuzzy logic differs from Boolean logic by associating every logical formula with a truth value in $[0, 1]$. Fuzzy logic systems usually retain the axioms of Boolean logic, which ensures that all logical operation behaviors are consistent with Boolean logic when the truth values are 0 or 1. Different fuzzy logic systems add different axioms to define the logical operation behavior for the case when the truth value is in $(0, 1)$ (Klir and Yuan 1995). A *t*-norm $\top : [0, 1] \times [0, 1] \mapsto [0, 1]$ represents generalized conjunction in fuzzy logic. Prominent examples of *t*-norms include Gödel *t*-norm $\top_{\min}\{x, y\} = \min(x, y)$, product *t*-norm $\top_{\text{prod}}\{x, y\} = xy$, and Łukasiewicz *t*-

$\text{norm}_{\text{Łukasiewicz}}^\top(x, y) = \max\{0, x + y - 1\}$, for $x, y \in [0, 1]$. Any other continuous t -norm can be described as an ordinal sum of these three basic ones (Klement, Mesiar, and Pap 2000). Analogously, t -conorm are dual to t -norms for disjunction in fuzzy logic – given a t -norm \top , the t -conorm is defined as $\perp(x, y) = 1 - \top(1 - x, 1 - y)$ based on De Morgan’s law and the negator $n(x) = 1 - x$ for $x, y \in [0, 1]$ (Klement, Mesiar, and Pap 2000). This technique inspired numerous subsequent works. For example, CQD (Arakelyan et al. 2021) uses t -norms and t -conorms to rank entities for query answering on KGs.

4 Methodology

In this section, we propose our model `FuzzQE`, a framework for answering FOL queries in the presence of missing edges. `FuzzQE` embeds entities as *stochastic vectors* and queries as *fuzzy vectors* (Katsaras and Liu 1977). Logical operators are implemented via fuzzy conjunction, fuzzy disjunction and fuzzy negation in the embedding space.

4.1 Queries and Entities in Fuzzy Space

Predicting whether an entity can answer a query means predicting the probability that the entity belongs to the answer set of this query. In our work, we embed queries and entities to the *fuzzy space* $[0, 1]^d$, a subspace of \mathbb{R}^d (Katsaras and Liu 1977).

Query embedding. Consider a query q and its fuzzy answer set S_q , its embedding \mathbf{S}_q is defined as a fuzzy vector $\mathbf{S}_q \in [0, 1]^d$ (Katsaras and Liu 1977). Intuitively, let Ω denote the universe of all the elements, and let $\{U_i\}_{i=1}^d$ denote a partition over Ω , i.e., $\Omega = \cup_{i=1}^d U_i$ and $U_i \cap U_j = \emptyset$ for $i \neq j$. Each dimension i of \mathbf{S}_q denotes the probability whether the corresponding subset U_i is part of the answer set S_q , i.e., $\mathbf{S}_q(i) = \Pr(U_i \subseteq S_q)$.

Entity embedding. For an entity e , we consider its embedding \mathbf{p}_e from the same fuzzy space. To model its uncertainty, we model it as a categorical distribution to fall into each subset U_i , namely, $\mathbf{p}_e \in [0, 1]^d$, $\mathbf{p}_e(i) = \Pr(e \in U_i)$, and $\sum_{i=1}^d \mathbf{p}_e(i) = 1$.

Score function. Accordingly, the score function $\phi(q, e)$ is defined as the expected probability that e belongs to the fuzzy set S_q :

$$\phi(q, e) = \mathbb{E}_{e \sim \mathbf{p}_e}[e \in S_q] = \sum_{i=1}^d \Pr(e \in U_i) \Pr(U_i \subseteq S_q) = \mathbf{S}_q^\top \mathbf{p}_e$$

Note for query embedding in `FuzzQE`, the all-one vector $\mathbf{1}$ represents the universe set (i.e. Ω), and the all-zero vector $\mathbf{0}$ represents an empty set \emptyset .

The above representation and scoring provides the following benefits: (i) The representation is endowed with probabilistic interpretation, and (ii) each dimension of the embedding vector is between $[0, 1]$, which satisfies the domain and range requirements of fuzzy logic and allows the model to execute element-wise fuzzy conjunction/disjunction/negation.

4.2 Relation Projection for Atomic Queries

Atomic queries like $q = \text{Compose}(\text{John Lennon}, V_?)$ serve as the building blocks to compute the complex queries. To embed atomic queries, we associate each relation $r \in \mathcal{R}$ with a projection operator \mathcal{P}_r , which is modeled by a neural network with a weight matrix $\mathbf{W}_r \in \mathbb{R}^{d \times d}$ and a bias vector $\mathbf{b}_r \in \mathbb{R}^d$, and transforms an anchor entity embedding \mathbf{p}_e into a query embedding:

$$\mathbf{S}_q = \mathcal{P}_r(\mathbf{p}_e) = \mathbf{g}(\text{LN}(\mathbf{W}_r \mathbf{p}_e + \mathbf{b}_r))$$

where LN is Layer Normalization (Ba, Kiros, and Hinton 2016), and $\mathbf{g} : \mathbb{R}^d \mapsto [0, 1]^d$ is a mapping function that constrains $\mathbf{S}_q \in [0, 1]^d$. Particularly, we consider two different choices for \mathbf{g} :

$$\text{Logistic function} : \mathbf{g}(\mathbf{x}) = \frac{1}{1 + e^{-(\mathbf{x})}}$$

$$\text{Bounded rectifier} : \mathbf{g}(\mathbf{x}) = \min(\max(\mathbf{x}, 0), 1)$$

We follow (Schlichtkrull et al. 2018) and adopt *basis-decomposition* to define \mathbf{W}_r and \mathbf{b}_r :

$$\mathbf{W}_r = \sum_{j=1}^K \alpha_{rj} \mathbf{M}_j; \quad \mathbf{b}_r = \sum_{j=1}^K \alpha_{rj} \mathbf{v}_j$$

Namely, \mathbf{W}_r as a linear combination of K basis transformations $\mathbf{M}_j \in \mathbb{R}^{d \times d}$ with coefficients α_{rj} that depend on r . Similarly, \mathbf{b}_r is a linear combination of K basis vectors $\mathbf{v}_j \in \mathbb{R}^d$ with coefficients α_{rj} . This form prevents the rapid growth in the number of parameters with the number of relations and alleviates overfitting on rare relations. It can be seen as a form of effective weight sharing among different relation types (Schlichtkrull et al. 2018). Atomic queries that project from one set to another can be embedded similarly.

In principle, any sufficiently expressive neural network or translation-based KG embedding model (Bordes et al. 2013; Ji et al. 2015) could also be employed as the relation projection operator in our framework.

4.3 Fuzzy Logic based Logical Operators

Fuzzy logic is mathematically equivalent to fuzzy set theory (Klir and Yuan 1995), with fuzzy conjunction equivalent to fuzzy set intersection, fuzzy disjunction equivalent to fuzzy set union, and fuzzy negation to fuzzy set complement. Fuzzy logic is thus used to define operations over fuzzy vectors. Particularly, we present `FuzzQE` with reference to product logic, one of the most prominent fuzzy logic systems (Klement, Mesiar, and Pap 2000). Alternative design choices based on Łukasiewicz and Gödel logic are discussed in Appendix G. The embeddings of $q_1 \wedge q_2$, $q_1 \vee q_2$, and $\neg q$ are computed as follows:

$$\begin{aligned} q_1 \wedge q_2 : \quad \mathcal{C}(\mathbf{S}_{q_1}, \mathbf{S}_{q_2}) &= \mathbf{S}_{q_1} \circ \mathbf{S}_{q_2} \\ q_1 \vee q_2 : \quad \mathcal{D}(\mathbf{S}_{q_1}, \mathbf{S}_{q_2}) &= \mathbf{S}_{q_1} + \mathbf{S}_{q_2} - \mathbf{S}_{q_1} \circ \mathbf{S}_{q_2} \\ \neg q : \quad \mathcal{N}(\mathbf{S}_q) &= \mathbf{1} - \mathbf{S}_q \end{aligned}$$

where \circ denotes element-wise multiplication (fuzzy conjunction), $\mathbf{1}$ is the all-ones vector, and $\mathcal{C}, \mathcal{D}, \mathcal{N}$ denote the embedding based logical operators respectively.

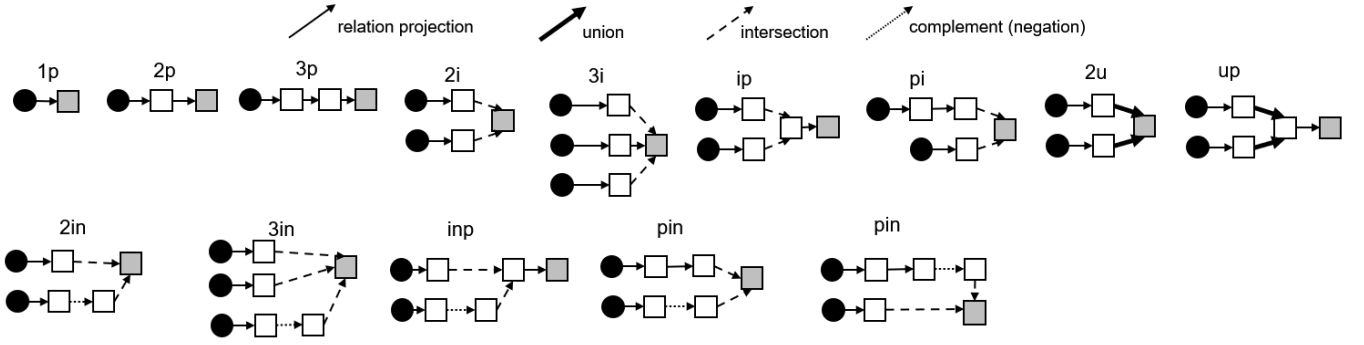


Figure 3: Query structure types used in training and evaluation. Naming convention: p for relation projection, i for conjunction (intersection), n for negation (complement), u for disjunction (union).

4.4 Model Learning and Inference

Given a query q , we optimize the following objective:

$$L = -\log \sigma(\phi(q, e) - \gamma) - \frac{1}{k} \sum_{i=1}^k \log \sigma(\gamma - \phi(q, e'_i))$$

where $e \in S_q$ is an answer to the query, $e' \notin S_q$ represents a random negative sample, and γ denotes the margin. In the loss function, we use k random negative samples and optimize the average. We seek to maximize $\phi(q, e)$ for $e \in S_q$ and minimize $\phi(q, e')$ for $e' \in S_q$.

For the model inference, given a query q , FuzzQE embeds it as S_q and rank all the entities by $\phi(q, \cdot)$.

4.5 Theoretical Analysis

For FuzzQE, we present the following propositions with proof in Appendix A.

Proposition 1. Our conjunction operator \mathcal{C} is commutative, associative, and satisfies conjunction elimination.

Proposition 2. Our disjunction operator \mathcal{D} is commutative, associative, and satisfies disjunction amplification.

Proposition 3. Our negation operator \mathcal{N} is involutory and satisfies non-contradiction.

5 Experiments

In this section, we evaluate the ability of FuzzQE to answer complex FOL queries over incomplete KGs.

5.1 Evaluation Setup

Datasets We evaluate our model on two benchmark datasets provided by (Ren and Leskovec 2020), which contain 14 types of logical queries on FB15k-237 (Toutanova and Chen 2015) and NELL995 (Xiong, Hoang, and Wang 2017) respectively. The 14 types of query structures in the datasets are shown in Fig. 3. Note that these datasets provided by BetaE (Ren and Leskovec 2020) are an improved and expanded version of the datasets provided by Query2Box (Ren, Hu, and Leskovec 2020). Compared to the earlier version, the new datasets Ren and Leskovec (2020) contain 5 new types of queries that involve negation. The

validation/test set of the original 9 query types are regenerated to ensure that the number of answers per query is not excessive, making this task more challenging. We exclude FB15k (Bordes et al. 2013) as this dataset suffers from major test leakage (Toutanova and Chen 2015). Details and statistics about the datasets are summarized in Appendix E.

Evaluation Protocol We follow the evaluation protocol in (Ren and Leskovec 2020). To evaluate the model’s generalization capability over incomplete KGs, the datasets are masked out so that each validation/test query answer pair involves imputing at least one missing edge. For each answer of a test query, we use the Mean Reciprocal Rank (MRR) as the major evaluation metric. We use the *filtered* setting (Bordes et al. 2013) and filter out other correct answers from ranking before calculating the MRR.

Baselines We consider three logical query embedding baselines for answering complex logical queries on KGs: GQE (Hamilton et al. 2018), Query2Box (Ren, Hu, and Leskovec 2020), and BetaE (Ren and Leskovec 2020). We also compare with one recent state-of-the-art query optimization model CQD (Arakelyan et al. 2021). For GQE, Query2Box, and BetaE we use implementation provided by (Ren and Leskovec 2020)³. For BetaE and CQD, we compare with the model variant that generally provides better performance, namely BetaE_{DNF} and CQD-BEAM. Note that CQD cannot process complex logical queries during training and is thus trained with KG edges. To the best of our knowledge, BetaE is the only available baseline that can handle negation. Therefore, for GQE, Query2Box, and CQD, we compare with them only on EPFO queries (queries with \exists, \wedge, \vee and without negation). We list the hyperparameters and more experimental details in Appendix F.

5.2 Main Results: Trained with FOL queries

We first test the ability of FuzzQE to model arbitrary FOL queries when complex logical queries are available for training. Results are reported in Table 3.

Comparison with Query Embedding As shown in Table 3, FuzzQE consistently outperforms all the logical

³<https://github.com/snap-stanford/KGReasoning>

Table 3: **MRR results (%) on answering FOL queries.** Report MRR results (%) on test FOL queries. Avg_{EPFO} and Avg_{Neg} denote the average MRR on EPFO queries (queries with \exists, \wedge, \vee and without negation) and queries containing negation respectively. Results of GQE, Query2Box, and BetaE are taken from (Ren and Leskovec 2020).

Type of Model	Model	Avg_{EPFO}	Avg_{Neg}	1p	2p	3p	2i	3i	pi	ip	2u	up	2in	3in	inp	pin	pni
FB15k-237																	
Query Embedding	GQE	16.3	N/A	35.0	7.2	5.3	23.3	34.6	16.5	10.7	8.2	5.7	N/A	N/A	N/A	N/A	N/A
	Query2Box	20.1	N/A	40.6	9.4	6.8	29.5	42.3	21.2	12.6	11.3	7.6	N/A	N/A	N/A	N/A	N/A
	BetaE	20.9	5.5	39.0	10.9	10.0	28.8	42.5	22.4	12.6	12.4	9.7	5.1	7.9	7.4	3.5	3.4
	FuzzQE	24.2	8.5	42.2	13.3	10.2	33.0	47.3	26.2	18.9	15.6	10.8	9.7	12.6	7.8	5.8	6.6
Query Optimization	CQD	21.7	N/A	46.3	9.9	5.9	31.7	41.3	21.8	15.8	14.2	8.6	N/A	N/A	N/A	N/A	N/A
NELL995																	
Query Embedding	GQE	18.6	N/A	32.8	11.9	9.6	27.5	35.2	18.4	14.4	8.5	8.8	N/A	N/A	N/A	N/A	N/A
	Query2Box	22.9	N/A	42.2	14.0	11.2	33.3	44.5	22.4	16.8	11.3	10.3	N/A	N/A	N/A	N/A	N/A
	BetaE	24.6	5.9	53.0	13.0	11.4	37.6	47.5	24.1	14.3	12.2	8.5	5.1	7.8	10.0	3.1	3.5
	FuzzQE	29.3	8.0	58.1	19.3	15.7	39.8	50.3	28.1	21.8	17.3	13.7	8.3	10.2	11.5	4.6	5.4
Query Optimization	CQD	28.4	N/A	60.0	16.5	10.4	40.4	49.6	28.6	20.8	16.8	12.6	N/A	N/A	N/A	N/A	N/A

Table 4: **MRR results (%) of logical query embedding models that are trained with only link prediction.** This task tests the ability of the model to generalize to arbitrary complex logical queries, when no complex logical query data is available for training. Avg_{EPFO} and Avg_{Neg} denote the average MRR on EPFO (\exists, \wedge, \vee) queries and queries containing negation respectively.

Model	Avg_{EPFO}	Avg_{Neg}	1p	2p	3p	2i	3i	pi	ip	2u	up	2in	3in	inp	pin	pni
FB15k-237																
GQE	17.7	N/A	41.6	7.9	5.4	25.0	33.6	16.3	10.9	11.9	6.2	N/A	N/A	N/A	N/A	N/A
Query2Box	18.2	N/A	42.6	6.9	4.7	27.3	36.8	17.5	11.1	11.7	5.5	N/A	N/A	N/A	N/A	N/A
BetaE	15.8	0.5	37.7	5.6	4.4	23.3	34.5	15.1	7.8	9.5	4.5	0.1	1.1	0.8	0.1	0.2
FuzzQE	21.8	6.6	44.0	10.8	8.6	32.3	41.4	22.7	15.1	13.5	8.7	7.7	9.5	7.0	4.1	4.7
NELL995																
GQE	21.7	N/A	47.2	12.7	9.3	30.6	37.0	20.6	16.1	12.6	9.6	N/A	N/A	N/A	N/A	N/A
Query2Box	21.6	N/A	47.6	12.5	8.7	30.7	36.5	20.5	16.0	12.7	9.6	N/A	N/A	N/A	N/A	N/A
BetaE	19.0	0.4	53.1	6.0	3.9	32.0	37.7	15.8	8.5	10.1	3.5	0.1	1.4	0.1	0.1	0.1
FuzzQE	27.1	7.3	57.6	17.2	13.3	38.2	41.5	27.0	19.4	16.9	12.7	9.1	8.3	8.9	4.4	5.6

query embedding baselines. For EPFO queries, FuzzQE improves the average MRR of best baseline BetaE (Ren and Leskovec 2020) by 3.3% (ca. 15% relative improvement) on FB15k-237 and 4.7% (ca. 19% relative improvement) on NELL995. For queries with negation, FuzzQE significantly outperforms the only available baseline BetaE. On average, FuzzQE improves the MRR by 3.0% (54% relatively) on FB15k-237 and 2.1% (36% relatively) on NELL995 for queries containing negation. We hypothesize that this significant enhancement comes from the principled design of our negation operator that satisfies the axioms, while BetaE fails to satisfy the non-contradiction property.

Comparison with Query Optimization: CQD We next compare FuzzQE with a recent query optimization baseline, CQD (Arakelyan et al. 2021) on EPFO queries. On average, FuzzQE provides 2.5% and 0.9% absolute improvement in MRR on FB15k-237 and NELL995 respectively. It is worth noting that FuzzQE outperforms CQD on most complex query structures on NELL995 even with slightly worse 1p performance. We hypothesize that the 1p perfor-

mance difference on NELL995 comes from the different ability of different relation projection/link prediction models to encode sparse graphs.

A major motivation for learning logical query embedding is its high inference efficiency. We compare with CQD with regard to the time for answering a query. On a NVIDIA[®] GP102 TITAN Xp (12GB), the average time for CQD to answer a FOL query on FB15k-237 is 13.9 ms (milliseconds), while FuzzQE takes only 0.3 ms. On NELL995, where the number of entities is 4 times the number in FB15k-237, the average time for CQD is 68.1 ms, whereas FuzzQE needs only 0.4 ms. CQD takes 170 times longer than FuzzQE. The reason is that CQD is required to score all the entities for each subquery to obtain the top- k candidates for beam search.

5.3 Trained with only Link Prediction

This experiment tests the ability of the model to generalize to arbitrary complex logical queries when it is trained with only the link prediction task. To evaluate it, we train

FuzzQE and other logical query embedding models using only KG edges (i.e. 1p queries). For baseline models GQE, Query2Box, and BetaE, we adapt them following the experiment settings of the Q2B-AVG-1P model discussed in (Ren, Hu, and Leskovec 2020). Specifically, we set all the sub-query weights to 1.0 for this experiment.

As shown in Table 4, FuzzQE is able to generalize to complex logical queries of new query structures even if it is trained on link prediction and provides significantly better performance than baseline models. Compared to the best baseline, FuzzQE improves the average MRR by 3.6% (20% relatively) for EPFO queries on FB15k-237 and 5.4% (26% relatively) on NELL995. Regarding queries with negation, our model drastically outperforms the only available baseline BetaE across datasets. In addition, compared with the ones trained with complex FOL queries (in Table 3), It is worth nothing that FuzzQE trained with only link prediction can outperform BetaE that are trained with extra complex logical queries (in Table 3). This demonstrates the superiority of the logical operators in FuzzQE, which are designed in a principled and learning-free manner. Meanwhile, FuzzQE can still take advantage of additional complex queries as training samples to enhance entity embeddings.

6 Conclusion

We propose a novel logical query embedding framework FuzzQE for answering complex logical queries on KGs. Our model FuzzQE borrows operations from fuzzy logic and implements logical operators in a principled and learning-free manner. Extensive experiments show the promising capability of FuzzQE on answering logical queries on KGs. The results are encouraging and suggest various extensions, including introducing logical rules into learning, as well as studying the potential use of predicate fuzzy logic systems and other deeper transformation architectures. Future research could also use the defined logical operators to incorporate logical rules to enhance reasoning on KGs. Furthermore, we are interested in jointly learning embeddings for logical queries, natural language questions, entity labels to enhance question answering on KGs.

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