Beta Embeddings for Multi-Hop Logical Reasoning in Knowledge Graphs

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Abstract

One of the fundamental problems in Artificial Intelligence is to perform complex multi-hop logical reasoning over the facts captured by a knowledge graph (KG). This problem is challenging, because KGs can be massive and incomplete. Recent approaches embed KG entities in a low dimensional space and then use these embeddings to find the answer entities. However, it remains a challenge to handle arbitrary first-order logic (FOL) queries as present methods are limited to only a subset of FOL operators. In particular, the negation operator is not supported. An additional limitation of present methods is also that they cannot naturally model uncertainty. Here, we present BetaE, a probabilistic embedding framework for answering arbitrary FOL queries over KGs. BetaE is the first method that can handle a complete set of first-order logical operations: conjunction ($\land$), disjunction ($\lor$), and negation ($\neg$). A key insight of BetaE is to use probabilistic distributions with bounded support, specifically the Beta distribution, and embed queries/entities as distributions, which allows us to also faithfully model uncertainty. Logical operations are performed in the embedding space by neural operators over the probabilistic embeddings. BetaE achieves state-of-the-art performance on answering arbitrary FOL queries on three large, incomplete KGs.

1. Introduction

Reasoning in KGs is a fundamental problem in AI. In essence, it involves answering first-order logic (FOL) queries over KGs using operators existential quantification ($\exists$), conjunction ($\land$), disjunction ($\lor$), and negation ($\neg$). It presents a number of significant challenges. One challenge is the scale of KGs. Although queries could be in principle answered by directly traversing the KG, this is problematic in practice since multi-hop reasoning involves an exponential growth in computational time/space. Another challenge is incompleteness, where some edges between entities are missing. Most real-world KGs are incomplete and even a single missing edge may make the query unanswerable.

Previous methods (Bordes et al., 2013; Trouillon et al., 2016; Sun et al., 2019; Zhang et al., 2019; Yang et al., 2015) aim to address the above challenges by using embeddings and this way implicitly impute the missing edges. Methods also embed logical queries into various geometric shapes in the vector space (Hamilton et al., 2018; Ren et al., 2020; Guu et al., 2015; Das et al., 2017). The idea here is to design neural logical operators and embed queries iteratively by executing logical operations according to the query computation graph (Fig. 1). However, these methods only support existential positive first-order queries, a subset of FOL queries with existential quantification ($\exists$), conjunction ($\land$) and disjunction ($\lor$), but not negation ($\neg$). Negation is a fundamental operation and required for the complete set of FOL operators. Modeling negation so far has been a major challenge. The reason is that these methods embed queries as closed regions, e.g., a point (Hamilton et al., 2018; Guu et al., 2015; Das et al., 2017) or a box (Ren et al., 2020) in the Euclidean space, but the complement (negation) of a closed region does not result in a closed region. Furthermore, current methods embed queries as static geometric shapes and are thus unable to faithfully model uncertainty.

Here we propose Beta Embedding (BetaE), a method for multi-hop reasoning over KGs using full first-order logic (FOL). We model both the entities and queries by probabilistic distributions with bounded support. Specifically, we embed entities and queries as Beta distributions defined on the $[0, 1]$ interval. Our approach has the following important advantages: (1) Probabilistic modeling can effectively capture the uncertainty of the queries. BetaE adaptively learns the parameters of the distributions so that the uncertainty of a given query correlates well with the differential entropy of the probabilistic embedding. (2) We design neural logical operators that operate over these Beta distributions and support full first-order logic: $\exists$, $\land$, $\lor$ and most importantly $\neg$. The intuition behind negation is that we can transform the parameters of the Beta distribution so that the regions of high probability density become regions of low probability.
We perform experiments on three standard KG datasets which provide the query answer. The disjunctive normal (directed) edges of relation type \( V \) allows \( \mathcal{B} \eta \alpha \) to handle a complete set of FOL operators and thus supporting arbitrary FOL queries.

We perform experiments on three standard KG datasets and show that \( \mathcal{B} \eta \alpha \) is able to achieve state-of-the-art performance in handling conjunctive queries and the first to handle arbitrary FOL logic queries in a scalable manner.

2. Preliminaries

Knowledge Graph (KG) \( \mathcal{G} \) is heterogeneous graph structure that consists of a set of entities \( \mathcal{V} \) and a set of relation types \( \mathcal{R} \), \( \mathcal{G} = (\mathcal{V}, \mathcal{R}) \). Each relation type \( r \in \mathcal{R} \) is a binary function \( r : \mathcal{V} \times \mathcal{V} \rightarrow \{\text{True}, \text{False}\} \) that indicates (directed) edges of relation type \( r \) between pairs of entities.

We are interested in answering first-order logic (FOL) queries with logical operations including conjunction (\( \land \)), disjunction (\( \lor \)), existential quantification (\( \exists \)) and negation (\( \neg \)). We define valid FOL queries in its disjunctive normal form (DNF), i.e., disjunction of conjunctions.

First-order logic queries: A FOL query \( q \) consists of a non-variable anchor entity set \( \mathcal{V}_0 \subseteq \mathcal{V} \), existentially quantified bound variables \( V_1, \ldots, V_k \) and a single target variable \( V_l \), which provides the query answer. The disjunctive normal form of a logical query \( q \) is a disjunction of one or more conjunctions: \( q[V_l] = V_l \land V_1 \lor \ldots \lor V_k \), where each \( c \) represents a conjunctive query with one or more literals \( e \). \( c = c_{11} \land c_{12} \land \ldots \land c_{1m} \); each literal \( e \) represents an atomic formula or its negation. \( e_{ij} = r(v_a, V) \lor \neg r(v_a, V) \lor r(V', V) \lor \neg r(V', V) \), where \( v_a \in \mathcal{V}_0 \), \( V \in \{V_l, V_1, \ldots, V_k\} \), \( V' \in \{V_1, \ldots, V_k\} \), \( r \in \mathcal{R} \).

Computation Graph: As shown in Fig. 1, we can derive, for a given query, its corresponding computation graph (tree). This directed graph demonstrates the computation process to answer the query. Each node of the computation graph represents a distribution over a set of entities in the KG and each edge represents a logical transformation of this distribution. Specifically, the root node represents the unique target variable, which is the set of answer entities. The mapping along each edge applies a certain logical operator: (1) Relation Projection: Given a set of entities \( S \subseteq \mathcal{V} \) and relation type \( r \in \mathcal{R} \), compute adjacent entities \( \bigcup_{v \in S} A_r(v) \) related to \( S \) via \( r: \bigcup_{v \in S} A_r(v) \equiv \{v' \in \mathcal{V} : r(v, v') = \text{True}\} \); (2) Intersection: Given sets of entities \( \{S_1, S_2, \ldots, S_n\} \), compute their intersection \( \bigcap_{i=1}^n S_i \); (3) Complement/Negation: Given a set of entities \( S \subseteq \mathcal{V} \), compute its complement \( \mathcal{S} \equiv \mathcal{V} \cup S \). We do not define a union operator for the computation graph, which corresponds to disjunction. However, this operator is not needed, since according to the De Morgan’s laws, given sets of entities, \( \bigcup_{i=1}^n S_i \equiv \mathcal{V} \cup S \). In order to answer a given FOL query, we can follow the computation graph and execute logical operators.

3. Probabilistic Embeddings for Reasoning

3.1. Beta Embeddings for Entities and Queries

For each entity \( v \in \mathcal{V} \), we assign an initial Beta embedding with learnable parameters. We also embed each query \( q \) with a Beta embedding, which is calculated by a set of probabilistic logical operators (introduced in the next section) following the computation graph. Note that \( \mathcal{B} \eta \alpha \) learns high-dimensional embeddings where each embedding consists of multiple independent Beta distributions, capturing a different aspect of a given entity or a query: \( S = [(\alpha_1, \beta_1), \ldots, (\alpha_n, \beta_n)] \), where \( n \) is a hyperparameter. We denote the PDF of the \( i \)-th Beta distribution in \( S \) as \( p_{B_{\alpha_i, \beta_i}} \). Without loss of generality and to ease explanation, we shall assume that each embedding only contains one Beta distribution: \( S = [(\alpha, \beta)] \), and we denote its PDF as \( p_{B_{\alpha, \beta}} \).
3.2. Probabilistic Logical Operators

In order to answer a query using the computation graph, we need probabilistic logical operators for the Beta embedding.

**Probabilistic Projection Operator** $P$: In order to model the relation projection from one distribution to another, we design a probabilistic projection operator $P$ that maps from one Beta embedding $S$ to another Beta embedding $S'$ given the relation type $r$. We then learn a transformation neural network for each relation type $r$, which we implement as a multi-layer perceptron (MLP): $S' = \text{MLP}_r(S)$. The goal here is that for all entities $S$ covered by the input distribution, we can achieve the embedding distribution that covers entities $S' = \cup_{v \in S} A_r(v)$, where $A_r(v) = \{v' \in V : r(v, v') = \text{True}\}$.

**Probabilistic Intersection Operator** $\mathcal{I}$: Given $n$ input embeddings $\{S_1, \ldots, S_n\}$, the goal of probabilistic intersection operator $\mathcal{I}$ is to calculate the Beta embedding $\mathbf{S}_{\text{Inter}}$ that represents the intersection of the distributions (i.e., the intersection of the distributions defining fuzzy input sets of entities). We model $\mathcal{I}$ by taking the weighted product of the PDFs of the input Beta embeddings $p_{\text{Inter}} = \frac{1}{Z} \prod p_{S_1}^{w_1} \cdots p_{S_n}^{w_n}$, where $Z$ is a normalization constant and $w_1, \ldots, w_n$ are the weights with their sum equal to 1.

We use the attention mechanism and learn $w_1, \ldots, w_n$ through a MLP that takes as input the parameters of $S_i$ and outputs a scalar. Since $S_i$ is a Beta distribution $[(\alpha_i, \beta_i)]$, the weighted product $p_{\text{Inter}}$ is a linear interpolation of the parameters of the inputs. We derive the parameters of $\mathbf{S}_{\text{Inter}}$ to be $[(\sum w_i \alpha_i), (\sum w_i \beta_i)]$:

$$p_{\text{Inter}}(x) \propto x^{\sum w_i (\alpha_i - 1)} (1 - x)^{\sum w_i (\beta_i - 1)} = x^{\sum w_i \alpha_i - 1} (1 - x)^{\sum w_i \beta_i - 1}$$

(1)

Our approach has three advantages (Fig. 2): (1) $\mathcal{I}$ demonstrates a zero-forcing behavior (Sun & Nielsen, 2019) where the effective support of $\mathbf{S}_{\text{Inter}}$ approximates the intersection of the effective support of the input embeddings. (2) $\mathcal{I}$ is closed, since the weighted product of PDFs of Beta distributions is proportional to a Beta distribution. (3) $\mathcal{I}$ is commutative w.r.t the input Beta embeddings.

**Probabilistic Negation Operator** $\mathcal{N}$: We require a probabilistic negation operator $\mathcal{N}$ that takes Beta embedding $S$ as input and produces an embedding of the complement $\mathcal{N}(S)$ as a result. A desired property of $\mathcal{N}$ is that the density function should reverse in the sense that regions of high density in $p_S$ should have low probability density in $p_{\mathcal{N}(S)}$ and vice versa (Fig. 2). For the Beta embeddings, this property can be achieved by taking the reciprocal of the shape parameters $\alpha$ and $\beta$: $\mathcal{N}([(\alpha, \beta)]) = [(1/\alpha, 1/\beta)]$. As shown in Fig. 2, the embeddings switch from bell-shaped unimodal density function with $1 < \alpha, \beta$ to bimodal density function with $0 < \alpha, \beta < 1$.

By defining the probabilistic logical operators $\mathcal{I}$ and $\mathcal{N}$, BETAE has the following properties: Given Beta embedding $S$, $S$ is a fixed point of $\mathcal{N} \circ \mathcal{I}$: $\mathcal{N}(\mathcal{I}(S, S, \ldots, S)) = S$. This shows that our design of the probabilistic intersection operator and the probabilistic negation operator achieves two important properties that obey the rules of real logical operations.

3.3. Learning Beta Embeddings

**Distance**: Assume each embedding consists of $n$ independent Beta distributions. Given an entity embedding $v$ with parameters $[(\alpha_1, \beta_1^1), \ldots, (\alpha_n, \beta_n^m)]$, and a query embedding $q$ with parameters $[(\alpha_q, \beta_q^1), \ldots, (\alpha_q, \beta_q^n)]$, we define the distance between this entity $v$ and the query $q$ as the sum of KL divergence between the two Beta embeddings along each dimension: $\text{Dist}(v; q) = \sum_{i=1}^{n} \text{KL}(p_{v,i}; p_{q,i})$, where $p_{s,i}$ represents the $i$-th Beta distribution.

**Training Objective**: Our objective is to minimize the distance between a query and its answers while maximizing the distance between the query and other random entities via negative sampling (Sun et al., 2019; Ren et al., 2020):

$$L = -\log \sigma (\gamma - \text{Dist}(v; q)) - \sum_{j=1}^{k} \frac{1}{k} \log \sigma (\text{Dist}(v'; q) - \gamma),$$

where $v \in [q]$ belongs to the answer set of $q$, $v' \notin [q]$ represents a random negative sample, and $\gamma$ denotes the margin. In the loss function, we use $k$ random negative samples and optimize the average.

4. Experiments

We evaluate BETAE on multi-hop reasoning over standard KGs. Our experiments demonstrate that: (1) BETAE effectively answers arbitrary FOL queries. (2) BETAE outperforms less general methods (Hamilton et al., 2018; Ren et al., 2020) on EPFO queries (with only $\exists$, $\land$ and $\lor$). (3) The probabilistic embeddings correspond well to the uncertainty.
We denote the rank as \( \text{H}@1 \) results (%) of \( \beta \text{E}, \text{Q}2\beta \) and \( \text{GQE} \) on answering \( \exists, \land, \lor \) queries.

### 4.1. Experiment Setup

Our experimental setup is focused on incomplete KGs and thus we measure performance only over answer entities that require (implicitly) imputing at least one edge. We use three standard KGs with official training/validation/test edge splits, FB15k (Bordes et al., 2013), FB15k-237 (Toutanova & Chen, 2015) and NELL995 (Xiong et al., 2017) and follow (Ren et al., 2020) for the preprocessing.

#### Evaluation Protocol

We first build three KGs: training KG, validation KG, test KG using training edges, training+validation edges, training+validation+test edges, respectively. Our evaluation focuses on incomplete KGs, so given a test (validation) query \( q \), we are interested in discovering non-trivial answers \( \langle q \rangle_{\text{test}} \lor \langle q \rangle_{\text{val}} \lor \langle q \rangle_{\text{train}} \). For each non-trivial answer \( r \) of a test query \( q \), we rank it against non-answer entities \( \lor \langle q \rangle_{\text{test}} \). We denote the rank as \( r \) and calculate the Mean Reciprocal Rank (MRR) and Hits at \( K \) (\( \text{H}@K \)) as evaluation metrics.

#### Queries

We base our queries on the 9 query structures proposed in Query2Box (\( \text{Q}2\beta \)) (Ren et al., 2020) and further create queries with negation. As shown in Fig. 3, we look at the 4 query structures with intersection (\( 2i/3i/ip/pi \)) and perturb one edge to perform set complement before taking the intersection, resulting in \( 2i/3i/\text{inp}/\text{pin} \) structures. See Appen. A for query generation details.

As summarized in Fig. 3, our training and evaluation queries consist of the 5 conjunctive structures (\( 1p/2p/3p/2i/3i \)) and also 5 novel structures with negation (\( 2i/3i/\text{inp}/\text{pin} \)). Furthermore, we also evaluate model’s generalization ability which means answering queries with structures that the model has never seen during training. We further include \( ip/pi/2u/up \) for evaluation.

#### Baselines

We consider two state-of-the-art baselines for answering complex logical queries on KGs: \( \text{Q}2\beta \) (Ren et al., 2020) and \( \text{GQE} \) (Hamilton et al., 2018). Both methods design their corresponding projection and intersection operators, however, neither can handle the negation operation since the complement of a point/box in the Euclidean space is no longer a point/box.

### 4.2. Modeling Arbitrary FOL Queries

**Modeling EPFO (containing only \( \exists, \land, \lor \)) Queries:** First we compare \( \beta \text{E} \) with baselines that can only model queries with conjunction and disjunction (but no negation). Table 2 shows the \( \text{H}@1 \) of the three methods. \( \beta \text{E} \) achieves on average 14.5%, 6.7% and 25.4% relative improvement \( \text{H}@1 \) over previous state-of-the-art \( \text{Q}2\beta \) on FB15k, FB15k-237 and NELL995, respectively. We refer the reader to Tables 8 in Appen. C for the MRR results.

### 4.3. Modeling the Uncertainty of Queries

We also investigate whether our \( \beta \text{E} \) embeddings are able to capture uncertainty. The uncertainty of a (fuzzy) set can be characterized by its cardinality. Given a query with answer set \([q]\), we aim to calculate the correlation between the differential entropy of the \( \beta \text{E} \) embedding \( p_{\text{en}} \) and the cardinality of the answer set \([q]\). For comparison, \( \text{Q}2\beta \) embeds each query as a box, which can also model the uncertainty of the query by expanding/shrinking the box size. Table 1 and Table 9 (in Appen. C) show that \( \beta \text{E} \) achieves up to 77% better correlation than \( \text{Q}2\beta \). We conclude that \( \beta \text{E} \) with \( \beta \text{E} \) embeddings is able to capture query uncertainty. Furthermore, note that \( \beta \text{E} \) naturally learns this property without any regularization to impose the correlation during training.
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A. Query Generation and Statistics

Generation of EPFO (with \( \exists, \lor \) and \( \land \)) Queries: Following (Ren et al., 2020), we generate the 9 EPFO query structures in a similar manner. Given the three KGs, and its training/validation/test edge splits, which is shown in Table 4, we first create \( G_{\text{train}}, G_{\text{valid}}, G_{\text{test}} \) as discussed in Sec. 4.1. Then for each query structure, we use pre-order traversal starting from the target node/answer to assign an entity/relation to each node/edge iteratively until we instantiate every anchor nodes (the root of the query structure). After the instantiation of a query, we could perform post-order traversal to achieve the answers of this query. And for validation/test queries, we explicitly filter out ones that do not exist non-trivial answers, i.e., they can be fully answered in \( G_{\text{train}}/G_{\text{valid}} \). Different from the dataset in (Ren et al., 2020), where the maximum number of test queries may exceed 5,000, we set a bar for the number of answers one query has, and additionally filter out unrealistic queries with more than 100 answers. We list the average number of answers the new test queries have in Table 5 and the number of training/validation/test queries in Table 6.

| Dataset    | Entities | Relations | Training Edges | Validation Edges | Test Edges | Total Edges |
|------------|----------|-----------|----------------|------------------|------------|-------------|
| FB15k      | 14,951   | 1,345     | 483,142        | 50,000           | 59,071     | 592,213     |
| FB15k-237  | 14,505   | 237       | 272,115        | 17,526           | 20,438     | 301,079     |
| NELL995    | 63,361   | 200       | 114,213        | 14,324           | 14,267     | 142,804     |

Table 4. Knowledge graph dataset statistics as well as training, validation and test edge splits.

| Dataset    | 1p | 2p | 3p | 2i | 3i | 1p | 2i | 3i | 1p |
|------------|----|----|----|----|----|----|----|----|----|
| FB15k      | 1.7| 19.6| 24.4| 8.0| 5.2| 18.3| 12.5| 18.9| 23.8|
| FB15k-237  | 1.7| 17.3| 24.3| 6.9| 4.5| 17.7| 10.4| 19.6| 24.3|
| NELL995    | 1.6| 14.9| 17.5| 5.7| 6.0| 17.4| 11.9| 14.9| 19.0|

Table 5. Average number of answers of test queries in our new dataset.

Generation of Queries with Negation: For the additional queries with negation, we derive 5 new query structures from the 9 EPFO structures. Specifically, as shown in Fig. 3, we only consider query structures with intersection for the derivation of queries with negation. The reason is that queries with negation are only realistic if we take negation with an intersection together. Consider the following example, where negation is not taken with intersection, “List all the entities on KG that is not European countries.”, then both “apple” and “computer” will be the answers. However, realistic queries will be like “List all the countries on KG that is not European countries.”, which requires an intersection operation. In this regard, We modify one edge of the intersection to further incorporate negation, thus we derive 2in from 2i, 3in from 3i, inp from ip, pin and pni from pi. Note that following the 9 EPFO structures, we also enforce that all queries with negation have at most 100 answers.

B. Experimental Details

We implement our code using Pytorch. We use the implementation of the two baselines GQE (Hamilton et al., 2018) and Q2B (Ren et al., 2020) in https://github.com/hyren/query2box. We finetune the hyperparameters for the three methods including number of embedding dimensions from \{200, 400, 800\} and the learning rate from \{1e^{-4}, 5e^{-3}, 1e^{-3}\}, batch size from \{128, 256, 512\}, and the negative sample size from \{32, 64, 128\}, the margin \( \gamma \) from \{20, 30, 40, 50, 60, 70\}. We list the hyperparameters of each model in the Table 7. Additionally, for our BETAE, we finetune the structure of the probabilistic projection operator MLP+, and the attention module MLPAtt. For both modules, we implement a three-layer MLP with 512 latent dimension and ReLU activation.
| Dataset       | Model | 1p  | 2p  | 3p  | 2i  | 3i  | pi  | ip  | 2u  | up  | avg  |
|---------------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| FB15k         | BetaE| 62.2| 24.6| 23.9| 52.5| 64.4| 41.3| 27.1| 36.8| 24.3| 39.7 |
|               | Q2B  | 67.1| 19.9| 13.5| 53.1| 64.4| 38.8| 24.9| 33.4| 15.7| 36.7 |
|               | GQE  | 54.6| 15.3| 10.8| 39.7| 51.4| 27.6| 19.1| 22.1| 11.6| 28.0 |
| FB15k-237     | BetaE| 38.2| 10.3| 9.7 | 27.3| 40.9| 21.1| 11.2| 11.7| 9.2 | 20.0 |
|               | Q2B  | 40.3| 9.1 | 6.6 | 28.8| 41.4| 21.0| 12.4| 10.6| 7.3 | 19.7 |
|               | GQE  | 35.0| 7.2 | 5.3 | 23.3| 34.6| 16.5| 10.7| 8.2 | 5.7 | 16.3 |
| NELL995       | BetaE| 52.5| 12.7| 11.0| 36.1| 46.8| 23.8| 13.9| 11.7| 8.6 | 24.1 |
|               | Q2B  | 41.8| 13.7| 10.9| 33.1| 43.9| 22.4| 16.7| 11.1| 9.7 | 22.6 |
|               | GQE  | 32.8| 11.9| 9.6 | 27.5| 35.2| 18.4| 14.4| 8.5 | 8.8 | 18.6 |

We run our method and two baselines for three times and report the average result with standard deviation. Each single experiment is run on a single NVIDIA GeForce RTX 2080 Ti GPU, and we run each method for 300k iterations.

C. Additional Experimental Results

We show in Table 8 the MRR results of the three methods on answering EPFO queries. Our methods show a significant improvement over the two baselines in all three datasets.

We show in Table 9 the Pearson correlation coefficient between the learned embedding and the number of answers of queries. Our method is better than the baseline Q2B in measuring the uncertainty of the queries.