Logic Embeddings for Complex Query Answering

Francois Luus 1 Prithviraj Sen 1 Pavan Kapanipathi 1 Ryan Riegel 1 Ndivhuwo Makondo 1 Thabang Lebese 1 Alexander Gray 1

Abstract

Answering logical queries over incomplete knowledge bases is challenging because: 1) it calls for implicit link prediction, and 2) brute force answering of existential first-order logic queries is exponential in the number of existential variables. Recent work of query embeddings provides fast querying, but most approaches model set logic with closed regions, so lack negation. Query embeddings that do support negation use densities that suffer drawbacks: 1) only improvise logic, 2) use expensive distributions, and 3) poorly model answer uncertainty. In this paper, we propose Logic Embeddings, a new approach to embedding complex queries that uses Skolemisation to eliminate existential variables for efficient querying. It supports negation, but improves on density approaches: 1) integrates well-studied t-norm logic and directly evaluates satisfiability, 2) simplifies modeling with truth values, and 3) models uncertainty with truth bounds. Logic Embeddings are competitively fast and accurate in query answering over large, incomplete knowledge graphs, outperform on negation queries, and in particular, provide improved modeling of answer uncertainty as evidenced by a superior correlation between answer set size and embedding entropy.

1. Introduction

Reasoning over knowledge bases is fundamental to Artificial Intelligence, but still challenging since most knowledge graphs (KGs) such as DBpedia (Bizer et al., 2009), Freebase (Bollacker et al., 2008), and NELL (Carlson et al., 2010) are often large and incomplete. Answering complex queries is an important use of KGs, but missing facts makes queries unanswerable under normal inference. Figure 1 shows an example of handling a logic query representing the natural language question “Which films star Golden Globe winners that have not also won an Oscar?” Answering this query involves multiple steps of KG traversal and existential first-order logic (FOL) operations, each producing intermediate entities. We consider queries involving missing facts, which means there is uncertainty about these intermediates that complicates the task. Two main approaches to answering such multi-hop queries involving missing facts are (i) sequential path search and (ii) query embeddings. Sequential path search grows exponentially in the number of hops, and requires approaches like reinforcement learning (Das et al., 2017) or beam search (Arakelyan et al., 2020) that have to explicitly track intermediate entities. Query embeddings prefer composition over search, for fast (sublinear) inference and tractable scaling to more complex queries. While relation functions have to learn knowledge, composition can otherwise use inductive bias to model logic operators directly to alleviate learning difficulty.

Query embeddings need to (a) predict missing knowledge, (b) model logic operations, and (c) model answer uncertainty. Query2Box models conjunction as intersection of boxes, but is unable to model negation as the complement of a closed region is not closed (Ren et al., 2020). Beta embeddings of (Ren & Leskovec, 2020) model conjunction as weighted interpolation of Beta distributions and negation as inversion of density, but improvise logic and depend on neural versions of logic conjunction for better accuracy. (Hamilton et al., 2018) models entities as points so are unable to naturally express uncertainty, while Query2Box uses poorly differentiable geometric shapes unsuited to uncertainty calculations. Beta embeddings naturally model uncertainty with densities and do support complex query embedding, although its densities have no closed form and entropy calculations are expensive.

Beta embeddings (Ren & Leskovec, 2020) are the first query embedding that supports negation and models uncertainty, however it (1) abruptly converts first-order logic to set logic, (2) only improvises set logic with densities, (3) requires expensive Beta distribution (no closed form), and (4) dis-similarity uses divergence that needs integration.

We present our logic embeddings to address these issues with (1) formulation of set logic in terms of first-order logic, (2) use of well-studied logic, (3) simple representation with truth bounds, and (4) fast, symmetric dissimilarity measure.

1IBM Research. https://github.com/francoisluus/KGReasoning

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Logic Embeddings for Complex Query Answering

Which films star Golden Globe winners that have not also won an Oscar?

Figure 1. Logic embeddings perform real-valued logic on latent propositions (latents), an array of truth bounds that describes any subset of entities. (a) A learnt Skolem function maps latents of singleton Oscar to latents of maximal subset of Oscar winners, and similarly for GoldenGlobe; (b) Complement of a subset is logical negation of latents that identify non-Oscar winners; (c) Intersection of subsets is logical conjunction of latents that identify “Golden Globe winners that have not also won an Oscar”; (d) $q(T) = 1 - D(T, A)$ measures logic satisfiability of candidate answer set directly, while nearest neighbors to intermediate embeddings can provide some explainability.

Figure 2. Computation graph for Figure 1 with product t-norm for intersect. Nodes are truth vectors that identify entity subsets. Embedding query logic reduces to a simple vectorized calculation.

Logic embeddings are a compositional query embedding with inductive bias of real-valued logic, for answering (with uncertainty) existential (∃) FOL multi-hop logical queries over incomplete KGs. It represents entity subsets with arrays of truth bounds on latent propositions that describe and compress their features and relations. This allows us to directly use real-valued logic to filter and identify answers. Truth bounds $[l, u]: 0 \leq l \leq u \leq 1$ from (Riegel et al., 2020) express uncertainty about truths, stating it can be a value range (e.g. unknown $[0, 1]$). Sum of bound widths model uncertainty, which correlates to answer size. Now intersection is simply conjunction ($\land$) of bounds to retain only shared propositions, union is disjunction ($\lor$) to retain all propositions, and complement is negation ($\neg$) of bounds to find subsets with opposing propositions.

The novelty of logic embeddings is that it (a) performs set logic with real-valued logic, (b) characterizes subsets with truth bounds, and (c) correlates bounds with uncertainty. Its benefits are (a) improved accuracy with well-studied t-norms, (b) faster, simplified calculations, and (c) improved prediction of answer size.

Our contributions of logic embeddings make several advances to address issues of poor logic and uncertainty modeling, and computational expense of current methods:

1. **Direct logic.** Defines Skolem set logic via maximal Skolemisation of first-order logic to embed queries, where proximity of logic embeddings directly evaluates logic satisfiability of first-order logic queries.

2. **Improved logic.** Performs set intersection as logic conjunction over latent propositions with t-norms, often used for intersection of fuzzy sets. (Mostert & Shields, 1957) decomposition provide weak, strong, and nilpotent conjunctions, which show higher accuracy than idempotent conjunction via density interpolation of (Ren & Leskovec, 2020).

3. **Direct uncertainty.** Truth bounds naturally model uncertainty and have fast entropy calculation. Both entropy and bounds width show superior correlation to answer size.

4. **Improved measure.** Measures dissimilarity with simple $L_1$-norm, which improves training speed and accuracy.

Our contributions also include (i) introduction of Skolem set logic in Section 2 to enable lifted inference, (ii) definition of logic embeddings in Section 3 to enable logic query composition, (iii) implementation details of method in Section 4, and (iv) detailed evaluation in Section 5 and new cardinality prediction experiment showing benefit of truth bounds.
2. Querying with Skolem set logic

We define an existential first-order language \( \mathcal{L} \) whose signature contains a set of functional symbols \( \mathcal{F} \) and a set of predicate symbols \( \mathcal{R} \). The alphabet of \( \mathcal{L} \) includes the logic symbols of conjunction (\( \land \)), disjunction (\( \lor \)), negation (\( \neg \)), and existential quantification (\( \exists \)). The semantics of \( \mathcal{L} \) interprets the domain of discourse as a family of subsets \( \mathcal{C} \subseteq 2^V \), where \( 2^V \) denotes the power set of a set of entities \( V \). This allows for lifted inference where variables and terms map to entity subsets, which are single elements in the discourse.

Sentences of \( \mathcal{L} \) express relational knowledge, e.g., a binary predicate \( r \in \mathcal{R} \) relates two unordered subsets via function \( r : \mathcal{C} \times \mathcal{C} \rightarrow \{0, 1\} \) that evaluates to a real truth value. However, the underlying knowledge is predicated under a different signature on domain of discourse \( \mathcal{V} \), relating entities via \( r' : \mathcal{V} \times \mathcal{V} \rightarrow \{\text{False}, \text{True}\} \). Subsets \( c, t \in \mathcal{C} \) are related via \( r(c, t) \), with the union \( t = \bigcup_{v \in c} r'(v, t') \) for all underlying propositions \( r'(v, t') \) for each entity \( v \in c \) (see Figure 5).

Existential quantification in \( \mathcal{L} \) results in sentences that are always true in the underlying interpretation, because the nullset is present in \( \mathcal{C} \). We introduce maximal quantification via a modified Skolem function to make \( \mathcal{L} \) useful.

**Definition 1** (Maximal Skolem function). A maximal Skolem function \( f_r \in \mathcal{F} : \mathcal{C} \rightarrow \mathcal{C} \) assigns the maximal subset \( c \) to an existentially quantified variable \( T \) so that \( \exists T.r(a, T) \leftrightarrow r(a, f_r(a)) \) (equisatisfiable). The function receives input element \( a \in \mathcal{C} \) and outputs the related subset \( c \) over \( V \) with the largest cardinality, so that \( f_r(a) = c : |c'| \leq |c|, c, \forall c' \in \mathcal{C} \).

![Figure 4. Computation and dependency graph for the pin query in Table 1, we map FOL to Skolem set logic with simple rules.](image)

![Figure 5. A maximum Skolem function relates subset \( c \) via \( r(c, t) \) to the largest subset \( t = \{t'_1, t'_2, t'_3\} \), and not to smaller subsets, e.g. \( \{c'_1\} \) or \( \{c'_1, c'_2\} \), even if these satisfy \( r'(v, t') \) \( : v \in c, t' \in t \).](image)

| First-order logic | Skolem set logic |
|-------------------|------------------|
| 1p                | \( \exists T.p(a, T) \) |
| 2p                | \( \exists V.T.p(a, V) \land q(V, T) \) |
| 3p                | \( \exists V.p(a, V) \land q(V, W) \land r(W, T) \) |
| 2i                | \( \exists T.p(a, T) \land q(b, T) \) |
| 3i                | \( \exists T.p(a, T) \land q(b, T) \land r(c, T) \) |
| pi                | \( \exists V.T.p(a, V) \land q(V(T)) \land r(b, T) \) |
| ip                | \( \exists V.T.p(a, V) \land q(V, T) \land r(W, T) \) |
| 2u                | \( \exists T.p(a, T) \lor q(b, T) \) |
| up                | \( \exists V.T.p(a, V) \lor q(b, V) \land r(V, T) \) |

Formulate \( \mathcal{L} \) such as \( \exists a.r(a, T) \) can thus convert to sentences \( \exists T.r(a, T) \) by quantification over free variables, and the largest satisfying assignment to target variable \( T : r(a, T) \) obtained via **maximal Skolemisation** \( f_r(a) \) then subsumes all valid groundings in the underlying interpretation over \( \mathcal{V} \). “Relation following” of (Cohen et al., 2020) is similar where \( \exists a.r(a, T) = \{t' | \exists a \in r'(v', T') \} \). Normal Skolem functions are different as they only map to single entities.

**Skolem set logic.** This is set logic that involves Skolem functions that substitute related subsets. We introduce notation for **maximal Skolemisation** of sentences in \( \mathcal{L} \) that represents set logic on Skolem terms in their underlying interpretation over \( \mathcal{V} \). Evaluation in \( \mathcal{L} \) of conjunction \( \land \), disjunction \( \lor \), and negation \( \neg \) correspond to intersection, union, and complement in Skolem set logic, respectively.2

Sentence forms and their Skolem set logic representations (\( \land, \lor \) extends trivially to more inputs) for target variable \( T \), given anchor elements \( a, b \) (assigned subsets) and relation predicates \( r, \ldots, z \) include these conversion rules:

- **Relation**: \( \exists T.r(a, T) \) gives \( f_r(a) \).
- **Negation**: \( \exists T.\neg r(a, T) \) gives \( \neg f_r(a) \).
- **Conjunction**: \( \exists T.r(a, T) \land q(b, T) \) gives \( f_r(a) \land f_q(b) \).
- **Disjunction**: \( \exists T.r(a, T) \lor q(b, T) \) gives \( f_r(a) \lor f_q(b) \).
- **Multi-hop**: \( \exists T.r(a, V_1) \land q(V_1, V_2) \land \ldots \land z(V_{n-1}, T) \) has chain-like relations that give \( f_z \cdots (f_q(f_r(a))) \).

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2Skolem set logic reuses operators \( \land, \lor, \neg \) to signify that it performs direct real-valued logic on truth vectors of its terms. Skolem set logic usages are noted to avoid confusion with FOL.
We recast formulae into $C$ by converting anchor entities to singleton subsets, we then quantify $T$ to maximally Skolemise the sentence and derive its Skolem set logic term $f(a_1,a_2,\ldots,a_m)$ for $T$ given the anchor entities.

The dependency graph of formula (1) consists of vertices $\{a_1,\ldots,a_m,V_1,\ldots,V_n\}$ and a directed edge for each vertex pair $(x,y)$ related inside the formula, e.g. via $r(x,y)$. Queries are valid when the dependency graph is a single-sink acyclic graph with anchor entities as source nodes (Hamilton et al., 2018), and an equivalent to the original formula can then be recovered from Skolem set logic.

### 3. Logic Embeddings

Our approach for positive inference on queries of form (1) require only Skolem set logic, but should also support:

1. **Lifted inference**: Inference over subsets of entities, needing fewer actions than with single-entity inference;
2. **Knowledge integration**: Underlying single-entity knowledge over $\mathcal{V}$ integrates over subsets from $\mathcal{C}$;
3. **Generalization**: Use of subset similarities to predict absent knowledge with an uncertainty measure.

The powerset $\mathcal{C}$ over entities $\mathcal{V}$ from a typical KB is extremely large, so discrete approaches to achieve above with non-uniform subset representations are likely intractable.

**Set embeddings.** We consider set embeddings that map $\mathcal{C}$ to a continuous space $\mathcal{M}$, so these images of subsets approximately preserve their relationships from $\mathcal{C}$ (Sun & Nielsen, 2019). It has metric properties such as the volume of subsets, not usually considered by graph embeddings. **Set embeddings** have the following properties:

- **Uniform**: Enables standard parameterization, simplifies memory structures and related computation;
- **Continuous**: Differentiable, enables optimization;
- **Permutation-invariant**: Subset elements unordered;
- **Uncertainty**: Subset size corresponds to entropy;
- **Proximity**: Relatively preserves subset dissimilarities.

**Definition 2** (Logic embeddings). **Logic embeddings** are set embeddings that characterize subsets with latent propositions, and perform set logic on subsets via logic directly over their latent propositions. 

Logic embeddings inherit the aforementioned properties and benefits of set embeddings, but are also:

- **Logical**: Logic over truth values in embeddings performs set logic, and proximity correlates with satisfiability;
- **Contextual**: Latent propositions integrate select knowledge depending on the subset;
- **Open-world**: Accepts and integrates unknown or partially known knowledge and inferences.

Logic embeddings also share query embedding advantages of efficient answering, generalization, and full logic support:

- **Fast querying**: Obtains answers closest to query embedding in sublinear time, unlike subgraph matching with exponential time in query size (Dalvi & Suciu, 2007).
- **General querying**: Generalizes to unseen query forms.
- **Implicit prediction**: Implicitly imputes missing relations, and avoids exhaustive link prediction (De Raedt, 2008) subgraph matching requires and scales poorly on.
- **Natural modeling**: Supports intuitive set intersection, unlike point embeddings (Hamilton et al., 2018).
- **Uncertainty**: Models answer size with embedding entropy (Ren & Leskovec, 2020) or truth bounds (Ours).
- **Fundamental support**: Handles negation (and disjunction via De Morgan’s law), unlike box embeddings where complements are not closed regions (and union resorts to disjunctive normal form) (Ren et al., 2020).

**Latent propositions.** A logic embedding keeps truth values with associate distribution $p_X \in \mathcal{M}$ on latent propositions of features and properties that characterize and distinguish subset $X \subset \mathcal{V}$. Subset entities $x \in X$ may share a similar relation $r(x,Y)$ to a particular subset $Y$, where latent propositions can integrate such identifying relations. Logic embeddings need to be contextual given the limited embedding capacity, as only some relations may be relevant to define a particular subset.

**Uncertainty.** We represent volume in embedding space with lower and upper bounds $[l,u]$ on truth values, to express uncertainty and allow correlation of embedding entropy of a subset with its cardinality. We use truth bounds of (Riegel et al., 2020) that admit the open-world assumption and have probabilistic semantics to interpret known ($l \leq u$), unknown ($[0,1]$) and contradictory states ($l > u$, not considered here).

The logic embedding for $X \subset \mathcal{V}$ is an $n$-tuple $S_X = ([l_1,u_1] : l_i, u_i \in [0,1])_{i=1}^n$ of lower and upper bounds pairs $(l_i \leq u_i)$ that represents an $n$-tuple $p_X = (P_i)_{i=1}^n$ of uniform distributions $P_i = U(l_i,u_i)$, which omits contradiction $l_i > u_i$. The chain rule for differential entropy $H(p_X) = H(P_1,\ldots,P_n)$ of the embedding distribution applies and gives an upper-bound in terms of components $H(P_i) = \log(u_i-l_i)$, where

$$H(P_1,\ldots,P_n) = \sum_{i=1}^n H(P_i | P_1,\ldots,P_{i-1}) \leq \sum_{i=1}^n H(P_i).$$
**Condition 1** (Uncertainty axiom). Set embeddings should (approx.) satisfy $\forall X \in C$: entropy $H(p_X)$ is a monotonically increasing function of $H(U_X)$, where $U_X$ is a uniform distribution over elements of $X$. \cite{SunNielsen2019}.

We measure adherence to the uncertainty axiom with correlation between subset size $|X|$ and entropy upper-bound $\sum_{i=1}^n H(P_i)$ or total truth interval width $\sum_{i=1}^n (u_i - l_i)$, and by predicting $|X|$ from $h_X = [H(P_i)]_{i=1}^n$.

**Proximity.** Subsets with high overlap should embed close by, whereas little to no overlap should result in relatively distant embeddings. We now review the proximity axiom.

**Condition 2** (Proximity axiom). $\forall (X, X') \in \mathcal{C}^2$: $D(p_X || p_{X'})$ should positively correlate with $D(U_X || U_{X'})$, given information divergence $D$ \cite{SunNielsen2019}.

Relative entropy is an important divergence where the family of $f$-divergences $D_f[p||q] = \int p(x) f(q(x)/p(x)) dx$ typically include log$(p(x))$ or $p(x)^{-1}$ terms over finite support $x \in X$. Uniform distributions $U(l, u)$ in logic embeddings may not cover $[0, 1]$ support, and may result in undefined divergence. Therefore, we measure dissimilarity $D(S_X, S_{X'}) \in [0, 1]$ between logic embeddings of subsets $(X, X')$ with the expected mean of $L$-norms of truth bounds, where

$$D(S_X, S_{X'}) = \sum_{i=1}^n \frac{|l_i - l'_i| + |u_i - u'_i|}{2n}.$$

**Condition 3** (Satisfiability axiom). Substitution instance $q(X')$ of first-order logic formula $q(T)$ has satisfiability $1 - D(S_X, S_{X'})$, where target variable $T$ has answer $X$.

Query $q(T)$ is true for answer $X$, since $1 - D(S_X, S_{X'}) = 1$, but candidate satisfiability $q(X')$ can reduce to minimum 0 (false), depending on the dissimilarity between $X'$ and $X$.

**Set logic.** Conjunction and disjunction of latent propositions of subsets perform their intersection and union, respectively, unlike information-geometric set embeddings that interpolate distributions. De Morgan’s law replaces conjunction $a \land b$ with conjunction and negations $\neg(\neg a \land \neg b)$. Invoke negation of $S = \neg(\neg S) = \{l_i, u_i\}_{i=1}^n$ describes complement $\neg S = \{1-u_i, 1-l_i\}_{i=1}^n$. We use continuous t-norm $\top : [0, 1]^k \mapsto [0, 1]$ to perform generalized conjunction for real-valued logic, and calculate $S' = \bigwedge_{j=1}^k S_j$ as

$$S' = \left(\bigwedge_{i=1}^k (T(\ell_i), \ldots, T(l_i^k)), T(u_i), \ldots, T(u_i^k))\right)_{i=1}^n.$$

\cite{MostertShields1957} decompose any continuous t-norm into Archimedean t-norms, namely minimum/Gödel $\top_{\text{min}}(t) = \min(t_1, \ldots, t_k)$, product $\top_{\text{prod}}(t) = \prod_{j=1}^k t_j$.

and Łukasiewicz $\top_{\text{lk}}(t) = \max(0, 1 - \sum_{j=1}^k (1 - t_j))$, which we evaluate separately to consider all prime aspects.

**Contextual.** Limited capacity requires intersection to reintegrate latent propositions contextually via a weighted t-norm:

1) continuous function $\top(w, t)$ of weights $w$ and truths $t$;
2) behaves equal to unweighted case if weights are 1; and
3) $w_j = 0$ removes input $j$, and weights are in $[0, 1]$.

$$\top_{\text{min}}(w, t) = \sum_{j=1}^{k} t_j w_j e^{\alpha t_j} \left/ \sum_{j=1}^{k} w_j e^{\alpha t_j} \right.$$

$$\top_{\text{prod}}(w, t) = \prod_{j=1}^{k} t_j^{w_j}$$

$$\top_{\text{lk}}(w, t) = \max \left(0, 1 - \sum_{j=1}^{k} w_j (1 - t_j) \right)$$

Weight $w_j^{(v)}$ for $(l_j^{(v)}, u_j^{(v)})$, the $j$th truth bounds in input $v$, depends on bounds of all conjunction inputs via attention, starting with function $g$ as

$$g_j^{(v)} = g(l_j^{(v)}, \ldots, l_j^{(v)}, u_j^{(v)}, \ldots, u_j^{(v)})$$

Softargmax over all the conjunction inputs yields a score $s_j^{(v)} = \exp(g_j^{(v)})/\sum_{j=1}^{k} \exp(g_j^{(v)})$ which normalizes after $w_j^{(v)} = s_j^{(v)} / \max(s_j^{(1)}, \ldots, s_j^{(k)})$ to ensure max weight 1.

### 4. Implementation

**Query embedding.** We calculate a logic embedding for a single-sink acyclic query with Skolem set logic over anchor entities. We keep vectors $\{r \in \mathbb{R}^d\}$ for relation embeddings, and $\{x \in [0, 1]^{2d}\}$ for logic embeddings of all entities, where $x = [l_1, \ldots, l_d, u_1, \ldots, u_d]$. To measure the “cost” of testing model uncertainty by tracking bounds we also test point truth embeddings $(l = u)$, where $x = [l_1, \ldots, t_d]$.

We parameterize our Skolem function $f_r(x) = f(r, x)$ with $F_1 \in \mathbb{R}^{3d \times h}$, $F_2 \in \mathbb{R}^{h \times h}$, and $F_3 \in \mathbb{R}^{h \times 2d}$ to relate $x$ to $y = [y_1, y_1', y'_u (1 - y_1)]$, where $[y_1, y'_u] = f'(r, x) = \sigma(\max(0, \max(0, [r, x] F_1)) F_2) F_3$ activates sigmoid.

Set logic has attention that uses $g(x) = \max(0, x G_1) G_2$ with parameter matrices $G_1 \in \mathbb{R}^{2d \times 2d}$ and $G_2 \in \mathbb{R}^{2d \times d}$.

**Cardinality prediction.** We predict the cardinality $|X|$ of subset $X$ from the entropy vector $h_X$ of its logic embedding with $\rho \cdot \sigma(\max(0, \max(0, h_X H_1) H_2) H_3)$ scaled by $\rho$, where $H_1 \in \mathbb{R}^{d \times \frac{d}{2}}$, $H_2 \in \mathbb{R}^{\frac{d}{2} \times \frac{d}{2}}$, and $H_3 \in \mathbb{R}^{\frac{d}{2} \times 1}$.

**Query answering.** Our objective is to embed a query $q$ relatively close to its answers $\{y\}$ and far from negative samples $\{z\}$. We train model parameters of 1 entity logic

\footnote{We use non-monotonic smoothmin $(\alpha = -10)$ for weighted minimum t-norm and set $l' = u' = (l + u)/2$ when $l > u$.}

\footnote{1:1 train:test, $\rho = 10^3$, 250 epochs, Adam opt. ($lr = 10^{-4}$).}

\footnote{Hyperparameters include $d = 400$, $h = 1600$, $\gamma = 0.375$, $k = 128$ random negative samples, 512 batch size, 450k epochs, Adam optimizer ($lr = 10^{-3}$). Pytorch on 1x NVIDIA Tesla V100.}
embeddings, 2) relation embeddings, 3) Skolem function, and 4) t-norm attention, to minimize query answering loss

\[- \log \sigma (\gamma - D(y, q)) - \sum_{j=1}^{k} \frac{1}{k} \log (D(z_j, q) - \gamma). \]  \( . (8) \]

5. Experiments

We primarily compare against Beta embeddings (BETA (Ren & Leskovec, 2020)) that also support arbitrary FOL queries and negation, where our logic embeddings (LOGIC with Łukasiewicz t-norm) show improved 1) generalization, 2) reasoning, 3) uncertainty modeling, and 4) training speed.

Datasets. We use two complex logical query datasets from: Q2B with 9 query structures (Ren et al., 2020), and BETA that adds 5 for negation (Ren & Leskovec, 2020). They generate random queries separately over three standard KGs with official train/valid/test splits, namely FB15k (Bordes et al., 2013), FB15k-237 (Toutanova & Chen, 2015), NELL995 (Xiong et al., 2017). Table 1 shows the first-order logic and Skolem set logic forms of the 14 query templates.

We separately follow the evaluation procedures of above Q2B and BETA datasets.7 Training omits ip/pi/2u/up (Table 1) to test handling of unseen query forms. Negation is challenging with 10x less queries than conjunctive ones.8

Generalization. Queries have at least one link prediction task to test generalization, where withheld data contain goal answers. We measure Hits@k and mean reciprocal rank (MRR) of these non-trivial answers that do not appear in train/valid data. Table 4 tests both disjunctive normal form (DNF) and De Morgan’s form (DM) for unions (2u/up), but we only report DNF elsewhere as it outperforms DM.

LOGIC with bounds generalizes better than BETA, Q2B, and GQE (Hamilton et al., 2018) on almost all query forms in Table 4, and further improves with point truths.3 LOGIC also answers negation queries more accurately than BETA for most query forms in Table 2. CQD-Beam does not handle negation nor uncertainty and is expensive as it grounds candidate entities explicitly, yet LOGIC generalizes better and more efficiently in Table 5(a) on FB15k-237 and NELL.

Reasoning. Logical entailment on queries without missing links tests how faithful deductive reasoning is. We thus train on all splits and measure entailment accuracy in Table 5(b). LOGIC on average reasons more faithfully than BETA, Q2B, and GQE baselines on all datasets.

EmQL is a query embedding that specifically optimises faithful reasoning (Sun et al., 2020), and thus outperforms all other methods in Table 5(b). However, EmQL without

1https://github.com/francoisluus/KGReasoning
2Please see appendix for statistics of datasets.
3Please see appendix for full results on FB15k and NELL.

Table 2. Test MRR results (% higher better) of LOGIC and BETA on answering queries with negation (BETA dataset).9

| Model   | FB15k-237 | FB15k | NELL | avg | avg | avg |
|---------|-----------|-------|------|-----|-----|-----|
| LOGIC   |           |       |      |     |     |     |
| +bounds | 4.9       | 8.2   | 7.7  | 3.6 | 3.5 | 5.6 |
| BETA    | 5.1       | 7.9   | 7.4  | 3.6 | 3.4 | 5.4 |

Table 3. Validation MRR averages (%) higher better for LOGIC with various t-norms and BETA on training queries (BETA datasets), where i, n, and p are all query forms containing intersection, negation, or relation components, respectively.

| Model   | FB15k-237 | NELL995 | avg | avg |
|---------|-----------|---------|-----|-----|
| +bounds |           |         |     |     |
| luk     | 14.4      | 5.0     | 13.2| 15.8| 18.8| 6.5| 19.5| 21.5| 18.7|
| min     | 14.4      | 5.0     | 13.2| 15.7| 18.6| 6.6| 19.4| 21.5| 18.6|
| prod    | 14.4      | 5.0     | 13.3| 15.8| 18.7| 6.6| 19.4| 21.5| 18.7|
| BETA    | 13.7      | 4.8     | 12.6| 15.0| 17.5| 6.1| 17.0| 19.6| 17.3|

its sketch method has worse faithfulness than LOGICE with point truths for FB15k and NELL, also EmQL does not support negation nor models uncertainty like LOGICE.

Compare logics. LOGICE can intersect via minimum, product, or Łukasiewicz t-norms, which perform similarly (±1%) in Table 3, while all outperform BETA. Łukasiewicz provides superior uncertainty modeling, so is the default choice for LOGICE. Attention via weighted t-norm improves LOGICE accuracy (+9.6%), where one hypothesis is better use of limited embedding capacity through learning weighted combinations of latent propositions.

However, BETA improves by avg. +12.3% with a similar attention mechanism so has greater dependence on it, possibly because it devises intersection as interpolation of densities, whereas LOGICE uses established real-valued logic via t-norms. In particular, the BETA intersect is idempotent while LOGICE offers weak and strong conjunctions of which Łukasiewicz offers nilpotency.

Uncertainty modeling. Correlation between differential entropy \( \sum_{i=1}^{n} H(P_i) \) (upper-bound) and answer size (uncertainty, number of entities) is significantly higher in LOGICE than BETA using both Spearman’s rank correlation and
Table 4. Test MRR results (%, higher better) of LOGIC, BETA, Q2B and GQE on answering EPFO (∃, ∧, ∨) queries (BETA dataset).\(^9\)

| Model  | 1p | 2p | 3p | 2i | 3i | pi | ip | 2u | DM | 10.2 | 9.8 | 22.3 | 44.1 | 28.6 |
|--------|----|----|----|----|----|----|----|----|----|------|-----|------|------|-----|
| LOGIC  | 41.3 | 11.8 | 10.4 | 31.4 | 43.9 | 23.8 | 14.0 | 13.4 | 13.1 | 10.2 | 9.8 | 22.3 | 44.1 | 28.6 |
| + bounds | 40.5 | 11.4 | 10.1 | 29.8 | 42.2 | 22.4 | 13.4 | 13.0 | 12.9 | 9.8 | 9.6 | 21.4 | 40.8 | 28.0 |
| BETA   | 39.0 | 10.9 | 10.0 | 28.8 | 42.5 | 22.4 | 12.6 | 12.4 | 11.1 | 9.7 | 9.9 | 20.9 | 41.6 | 24.6 |
| Q2B    | 40.6 | 9.4  | 6.8  | 29.5 | 42.3 | 21.2 | 12.6 | 11.3 | 7.6  | 7.6  | 20.1 | 38.0 | 22.9 |
| GQE    | 35.0 | 7.2  | 5.3  | 23.3 | 34.6 | 16.5 | 10.7 | 8.2  | 5.7  | 16.3 | 16.3 | 28.0 | 18.6 |

Table 5. Hits@3 results (higher better) on the Q2B datasets testing (a) generalization and (b) reasoning faithfulness.\(^9\)

| Model  | 1p | 2p | 3p | 2i | 3i | pi | ip | 2u | DM | avg | avg | avg |
|--------|----|----|----|----|----|----|----|----|----|-----|-----|-----|
| LOGIC  | 46.1 | 28.6 | 24.8 | 34.8 | 46.5 | 12.0 | 23.7 | 27.7 | 21.1 | 29.5 | 54.9 | 39.3 |
| + bounds | 45.0 | 26.6 | 23.0 | 32.0 | 44.1 | 11.1 | 22.1 | 25.5 | 20.4 | 27.7 | 50.3 | 38.6 |
| EmQL   | 37.7 | 34.3 | 34.3 | 44.3 | 49.4 | 40.8 | 42.3 | 8.7  | 28.2 | 35.8 | 49.5 | 46.8 |
| CQD-Beam | 43.1 | 25.3 | 22.3 | 31.3 | 44.6 | 10.2 | 22.3 | 26.6 | 18.0 | 27.1 | 51.4 | 33.8 |
| BETA   | 46.7 | 24.0 | 18.6 | 32.4 | 45.3 | 10.8 | 20.5 | 23.9 | 19.3 | 26.8 | 48.4 | 30.6 |
| GQE    | 40.5 | 21.3 | 15.5 | 29.8 | 41.1 | 8.5  | 18.2 | 16.9 | 16.3 | 23.1 | 38.7 | 24.8 |

Table 6. Spearman’s rank correlation and Pearson’s correlation coefficient (higher better) between learned embedding (diff. entropy and truth interval width for LOGIC, diff. entropy for BETA, L1 box size for Q2B) and the number of answers of queries (BETA dataset).\(^9\)

| Model  | 1p | 2p | 3p | 2i | 3i | pi | ip | 2u | DM | avg | avg | avg |
|--------|----|----|----|----|----|----|----|----|----|-----|-----|-----|
| LOGIC  | 0.65 | 0.67 | 0.72 | 0.61 | 0.51 | 0.57 | 0.60 | 0.69 | 0.54 | 0.62 | 0.61 | 0.67 | 0.62 | 0.58 | 0.61 |
| + bounds | 0.61 | 0.58 | 0.58 | 0.64 | 0.64 | 0.54 | 0.49 | 0.58 | 0.50 | 0.41 | 0.49 | 0.60 | 0.56 | 0.51 | 0.53 |
| EmQL   | 0.40 | 0.50 | 0.57 | 0.60 | 0.52 | 0.54 | 0.44 | 0.69 | 0.58 | 0.51 | 0.47 | 0.67 | 0.54 | 0.49 | 0.55 |
| BETA   | 0.18 | 0.23 | 0.27 | 0.35 | 0.44 | 0.36 | 0.20 | -   | -   | -   | -   | -   | -   | -   | -   |

Table 7. Answer size prediction mean absolute error (%, lower better) with embedding entropy components for LOGIC and BETA, and box size components for Q2B (BETA dataset).\(^9\)

| Model  | 1p | 2p | 3p | 2i | 3i | pi | ip | 2u | DM | avg | avg | avg |
|--------|----|----|----|----|----|----|----|----|----|-----|-----|-----|
| LOGIC  | 78  | 83  | 86  | 82  | 94  | 89  | 86  | 81  | 79  | 81  | 81  | 83  | 87  | 80  |
| BETA   | 111 | 96  | 97  | 97  | 97  | 95  | 97  | 97  | 95  | 97  | 97  | 98  | 95  | 95  |
| Q2B    | 191 | 101 | 100 | 310 | 780 | 263 | 103 | -   | -   | -   | -   | -   | -   | -   |
Figure 6. Test accuracy vs. training time comparison (V100).

Pearson’s correlation coefficient in Table 6. Both significantly outperform uncertainty of Q2B with $L_1$ box size.

Total truth interval width $\sum_{i=1}^{n}(u_i - l_i)$ of LOGIC E correlates better to answer size in most cases than BETAE, and offers direct use of the probabilistic semantics of truth bounds to simplify uncertainty modeling. Note that minimizing query answering loss in Eq. (8) does not directly optimize answer cardinality, so LOGIC E naturally models uncertainty only as by-product of learning to answer.

Cardinality prediction. Above evaluation aggregates entropy, but element-wise entropies $h_X = \frac{1}{n} \sum_{j=1}^{n} h_i$ contain more information that we use for explicit answer size prediction. We train a regression classifier to map provided uncertainties $h_X$ to answer size $|X|$, and measure mean absolute error $\|s - |X||/|X|$ of size prediction $s$.

Table 7 shows reduced cardinality prediction error of 83% with LOGIC E, compared to avg. 96% with BETAE, indicating more informative uncertainties with LOGIC E. However, these errors are still quite large, possibly because the main training objective does not directly optimize uncertainties for cardinality prediction.

Training speed. BETAE uses the Beta distribution with no closed form that requires integration to compute entropy and dissimilarity. In contrast, LOGIC E uses simple truth bounds with fast entropy and dissimilarity calculations. Figure 6 shows that LOGIC E with any t-norm trains 2-3x faster than BETAE, with the exact same compute resources, optimizer and learning rate. The LOGIC E training curve also appears smooth and monotonic, compared to disrupted learning progress with BETAE.

6. Related work

In addition to the overview of query embeddings in the Introduction, we also relate our work to 1) tensorized logic, 2) querying with t-norms, and 3) lifted inference.10

Tensorized logic. Distributed representations like embeddings can enable generalization and efficient inference that symbolic logic lacks. Logic tensors of (Grefenstette, 2013) express truths as specific tensors and map entities to one-hot vectors with full-rank matrices, but only memorize facts. Matrix factorization reduces one-hot vectors to low dimensions to enable generalization and efficiency while optimizing logic constraints, but can scale exponentially in the number of query variables (Rocktäschel et al., 2015).

Logic Tensor Networks learn a real vector per entity and even Skolem functions that map to entity features, but has weak inductive bias as it needs to learn predicates to perform logic (Serafini & Garcez, 2016). In contrast, logic embeddings support uncertainty and only has to learn Skolem functions to express knowledge and generalize, with direct logic on latent truths and logic satisfiability via distance.

Querying with t-norms. Triangular norms allow for differentiable composition of scores, often in the context of expensive search. (Guo et al., 2016) jointly embed KGs and logic rules via t-norm of scores, but only for simple rules. (Arakelyan et al., 2020) combine scores from a pretrained link predictor via t-norms repeatedly to search for an answer while tracking intermediaries, whereas logic embeddings perform vectorized t-norm to directly embed answers.

Lifted inference. Many probabilistic inference algorithms accept first-order specifications, but perform inference on a mostly propositional level by instantiating first-order constructs (Friedman et al., 1999; Richardson & Domingos, 2006). In contrast, lifted inference operates directly on first-order representations, manipulating not only individuals but also groups of individuals, which has the potential to significantly speed up inference (de Salvo Braz et al., 2007). We need to reason about entities we know about, as well as those we know exist but with unknown properties. Logic embeddings perform a type of lifted inference as it does not have to ground out the theory or reason separately for each entity, but can perform logic inference directly on subsets.

7. Conclusion

Embedding complex logic queries close to answers is efficient but presents several difficulties in set theoretic modeling of uncertainty and full existential FOL, where Euclidean geometry and probability density approaches suffer deficiency and computational expense. Our logic embeddings overcome these difficulties by converting set logic into direct

10Please see appendix for an extended related work section.
real-valued logic. We execute FOL queries logically, and not through Venn diagram models like other embeddings, yet we achieve efficiency of lifted inference over subsets.

Main limitations include the need for more training data than search-based methods, although we have strong inductive bias of t-norm logic to reduce sample size dependence. Future work will consider negation attending to applied relations of its input to benefit from context like the t-norms.

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A. Extended Related Work

Link prediction. Reasoning over knowledge bases is fundamental to Artificial Intelligence, but still challenging since most knowledge graphs (KGs) such as DBpedia (Bizer et al., 2009), Freebase (Bollacker et al., 2008), and NELL (Carlson et al., 2010) are often large and incomplete. Answering complex queries is an important use of KGs, but missing facts makes queries unanswerable under normal inference. KG embeddings are popular for predicting facts, learning entities as vectors and relations between them as functions in vector space, like translation (Bordes et al., 2013) or rotation (Sun et al., 2019).

Link prediction uncovers similar behavior of entities, and semantic similarity between relations (e.g. birthplace predicts nationality). Path queries involve multi-hop reasoning (e.g. country of birth of person), where compositional learning embeds queries close to answer entities with fast (sublinear) neighbor search (Guu et al., 2015). In contrast, sequential path search grows exponentially in the number of hops, and requires approaches like reinforcement learning (Das et al., 2017) or beam search (Arakelyan et al., 2020) that have to explicitly track intermediate entities.

Path-based methods. A simple approach to complex query answering represents first-order logical queries as a directed graph corresponding to the reasoning path to be followed. Such path-based methods are characterized by carrying out a sub-graph matching strategy in their pursuit for solving complex queries. However, they fail to deal with queries with missing relations and cannot scale to large KGs as the complexity of sub-graph matching grows exponentially in the query size. Several works aim at addressing the former by imputing missing relations (Guu et al., 2015; Hong et al., 2018), leading into a denser KG with high computational demand.

Query embeddings. Recent approaches aim to address the two issues by learning embeddings of the query such that entities that answer the query are close to the embeddings of the query and answers can be found by fast nearest neighbor searches. Such approaches implicitly impute missing relations and also lead to faster querying compared to subgraph matching. Here, logical queries as well as KG entities are embedded into a lower-dimensional vector space as geometric shapes such as points (Hamilton et al., 2018), boxes (Ren et al., 2020) and distributions with bounded support (Ren & Leskovec, 2020).

Compared to point-based embeddings, boxes and distributions naturally model sets of entities they enclose, with set operations on those sets corresponding to logical operations (e.g., set intersection corresponds to the conjunction operator), and thus iteratively executing set operations results in logical reasoning. Furthermore, box and distribution-based
embeddings allow handling the uncertainty over the queries. Majority of early embedding based approaches are limited to a subset of first-order logic consisting of existential quantification and conjunctions, with a few recent papers supporting the so-called existential positive first-order (EPFO) queries (Ren et al., 2020; Arakelyan et al., 2020) that additionally include disjunctions. The work by (Ren & Leskovec, 2020) is the first to handle the full set of first-order logic including negation.

Recent path-based approaches utilize knowledge graph embeddings to learn to tractably traverse the graph in the embedding space (Lou et al., 2020) or using pre-trained black boxes for link prediction (Arakelyan et al., 2020). Neural Subgraph Matching (Lou et al., 2020) uses order embeddings to embed the query and KG graphs into a lower-dimensional space, and efficiently performs subgraph matching directly in the embedding space. This has the potential to impute missing relations and has been shown to be orders of magnitude faster than standard sub-graph matching approaches on subgraph matching benchmarks. However, it has not been applied to complex query answering problems. (Arakelyan et al., 2020) use a pre-trained, black-box, neural link predictor to reduce sample complexity and scale to larger KGs, and was shown to be effective on EPFO queries, but does not support the full set of first-order logic queries.

Lifted inference. Many probabilistic inference algorithms accept first-order specifications, but perform inference on a mostly propositional level by instantiating first-order constructs (Friedman et al., 1999; Richardson & Domingos, 2006). In contrast, lifted inference operates directly on first-order representations, manipulating not only individuals but also groups of individuals, which has the potential to significantly speed up inference (de Salvo Braz et al., 2007).

Variable elimination of non-observed non-query variables is the basis of several lifted inference algorithms (Poole, 2003; de Salvo Braz et al., 2007), and strongly resembles the lifting lemma which simulates ground resolution because it is complete and then lifts the resolution proof to the first-order world (Chang & Lee, 2014).

Theorem proving produces a potentially unbounded number of resolutions on grounded representations by performing unification and resolution on clauses with free variables, operating directly on the first-order representation. However, reasoning over incomplete knowledge requires generalization where particular facts about some individuals could apply with uncertainty to a similar group, thus predicting missing facts.

We need to reason about entities we know about, as well as entities we know exist but which have unknown properties. Logic embeddings perform a type of lifted inference as it does not have to ground out the theory or reason separately for each entity, but can perform logic inference directly with compact representations of smooth sets of entities.

B. Query forms

Table 9 gives logic query forms from (Ren & Leskovec, 2020) with corresponding Skolem normal form and Skolem set logic. Note that Skolem normal form uses conventional set logic symbols inside predicates, to avoid confusion with logic symbols composing predicates. Subsequent Skolem set logic resumes use of logic symbols, as the actual operations are logical over vectors of truth values.

C. Dataset statistics

Table 10 gives the relation and entity counts, as well as the train/valid/test split edge counts for the three datasets used. Table 11 gives the number of generated queries for the Q2B query datasets, and Table 12 gives the query counts for the BETA query datasets.

D. Additional Results

Table 8 compares test MRR results for LOGIC and BETA on different datasets. Table 13 compares test MRR results for queries without negation. Table 14 provides full details of Spearman’s rank correlation for all three KGs. Table 15 gives full numbers on Pearson’s correlation coefficient for all three KGs. Table 16 gives answer size prediction mean absolute error for all three KGs. Table 17 provides generalization and entailment scores for all three KGs.

Table 8. Test MRR results (%) of LOGIC and BETA on answering queries with negation.

| Dataset  | Model  | 2in | 3in | inp | pin | pni | avg  |
|----------|--------|-----|-----|-----|-----|-----|------|
| FB15k    | LOGIC  | 15.1| 14.2| 12.5| 7.1 | 13.4| 12.5 |
|          | +bounds| 14.0| 13.4| 11.9| 6.6 | 12.4| 11.7 |
|          | BETA   | 14.3| 14.7| 11.5| 6.5 | 12.4| 11.8 |
| FB15k-237| LOGIC  | 4.9 | 8.2 | 7.7 | 3.6 | 3.5 | 5.6  |
|          | +bounds| 4.9 | 8.0 | 7.3 | 3.6 | 3.5 | 5.5  |
|          | BETA   | 5.1 | 7.9 | 7.4 | 3.6 | 3.4 | 5.4  |
| NELL995  | LOGIC  | 5.3 | 7.5 | 11.1| 3.3 | 3.8 | 6.2  |
|          | +bounds| 5.3 | 7.8 | 11.1| 3.3 | 3.8 | 6.3  |
|          | BETA   | 5.1 | 7.8 | 10.0| 3.1 | 3.5 | 5.9  |
Table 9. Complex logical query structures of (Ren & Leskovec, 2020) in first-order logic and Skolem set logic form.

| First-order logic | Skolem normal form | Skolem set logic |
|-------------------|--------------------|------------------|
| 1p $\exists T. p(a, T)$ | $p(a, f_p(a))$ | $f_p(a)$ |
| 2p $\forall V, T. p(a, V) \land q(V, T)$ | $p(a, f_p(a)) \land q(f_p(a), f_q(f_p(a)))$ | $f_p(a) \land f_q(f_p(a))$ |
| 3p $\exists V, W. T. p(a, V) \land q(V, W) \land r(W, T)$ | $p(a, f_p(a)) \land q(f_p(a), f_q(f_p(a))) \land r(f_q(f_p(a)), f_r(f_q(f_p(a))))$ | $f_p(a) \land f_q(f_p(a)) \land f_r(f_q(f_p(a)))$ |
| 2i $\exists T. p(a, T) \land q(b, T)$ | $p(a, f_p(a)) \land q(b, f_q(b))$ | $f_p(a) \land f_q(b)$ |
| 3i $\exists T. p(a, T) \land q(b, T) \land r(c, T)$ | $p(a, f_p(a)) \land q(b, f_q(b)) \land r(c, f_r(c))$ | $f_p(a) \land f_q(b) \land f_r(c)$ |
| pi $\forall V, T. p(a, V) \land q(V, T) \land r(b, T)$ | $p(a, f_p(a)) \land q(f_p(a), f_q(f_p(a))) \land r(b, f_r(b))$ | $f_p(a) \land f_q(f_p(a)) \land f_r(b)$ |
| ip $\forall V, T. [p(a, V) \land q(b, V)] \land r(V, T)$ | $[p(a, f_p(a)) \land q(b, f_q(b))] \land r(f_p(a) \land f_q(b))$ | $f_p(a) \land f_q(b)$ |
| 2u $\exists T. p(a, T) \lor q(b, T)$ | $p(a, f_p(a)) \lor q(b, f_q(b))$ | $f_p(a) \lor f_q(b)$ |
| up $\forall V, T. [p(a, V) \lor q(b, V)] \land r(V, T)$ | $[p(a, f_p(a)) \lor q(b, f_q(b))] \land r(f_p(a) \lor f_q(b))$ | $f_p(a) \lor f_q(b)$ |

Table 10. Dataset statistics according to (Ren & Leskovec, 2020) with training, validation and test edge splits.

| Dataset | Relations | Entities | Training Edges | Validation Edges | Test Edges | Total Edges |
|---------|-----------|----------|----------------|------------------|------------|-------------|
| FB15k   | 1.345     | 14,951   | 483,142        | 50,000           | 59,071     | 592,213     |
| FB15k-237 | 237      | 14,505   | 272,115        | 17,526           | 20,438     | 310,079     |
| NELL995 | 200       | 63,361   | 114,213        | 14,324           | 14,267     | 142,804     |

Table 11. Number of queries in Q2B dataset generated for different query structures (see Ren et al., 2020).

| Dataset | Training | Validation | Test |
|---------|----------|------------|------|
|         | lp others| lp others  | lp others |
| FB15k   | 273,710  | 59,097     | 67,016 |
| FB15k-237 | 149,689 | 20,101     | 22,812 |
| NELL995 | 107,982  | 16,927     | 17,034 |

Table 12. Number of queries in BETAE dataset generated for different query structures (see Ren & Leskovec, 2020).

| Dataset | Training | Validation | Test |
|---------|----------|------------|------|
|         | lp/2p/3p/2i/3i | lp/2p/3p/2i/3i | lp/2p/3p/2i/3i |
| FB15k   | 273,710  | 59,097     | 67,016 |
| FB15k-237 | 149,689 | 20,101     | 22,812 |
| NELL995 | 107,982  | 16,927     | 17,034 |
### Table 13. Test MRR results (%) of LOGICE, BETA, Q2B and GQE on answering EPFO (∃, ∧, ∨) queries (BETA data).

| Dataset     | Model       | 1p | 2p | 3p | 2i | 3i | pi | ip | 2in | 3in | inp | pin | pni | avg  |
|-------------|-------------|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|------|
| FB15k-237   | LOGICE+bounds | 0.52 | 0.57 | 0.60 | 0.63 | 0.56 | 0.71 | 0.58 | 0.59 | 0.67 | -   | -   | -   | 0.62 |
|             | LOGICE      | 0.37 | 0.40 | 0.47 | 0.50 | 0.42 | 0.53 | 0.48 | 0.50 | 0.59 | -   | -   | -   | 0.53 |
|             | BETA        | 0.40 | 0.50 | 0.57 | 0.47 | 0.50 | 0.54 | 0.44 | 0.50 | 0.57 | -   | -   | -   | 0.56 |
|             | Q2B         | 0.18 | 0.23 | 0.27 | 0.35 | 0.40 | 0.36 | 0.27 | 0.29 | 0.34 | -   | -   | -   | 0.56 |
| NELL995     | LOGICE+bounds | 0.67 | 0.64 | 0.60 | 0.63 | 0.55 | 0.70 | 0.59 | 0.59 | 0.49 | 0.55 | 0.70 | 0.61 | 0.61 |
|             | LOGICE      | 0.51 | 0.56 | 0.48 | 0.68 | 0.67 | 0.56 | 0.61 | 0.30 | 0.34 | 0.58 | 0.53 | 0.58 | 0.53 |
|             | BETA        | 0.42 | 0.55 | 0.56 | 0.59 | 0.61 | 0.60 | 0.54 | 0.30 | 0.34 | 0.58 | 0.53 | 0.58 | 0.53 |
|             | Q2B         | 0.15 | 0.29 | 0.31 | 0.38 | 0.41 | 0.36 | 0.35 | 0.30 | 0.34 | 0.58 | 0.53 | 0.58 | 0.53 |

### Table 14. Spearman’s rank correlation (higher better) between learned embedding (diff. entropy and truth intervals for LOGICE, diff. entropy for BETA, box size for Q2B) and the number of answers of queries.

| Dataset     | Model       | 1p | 2p | 3p | 2i | 3i | pi | ip | 2in | 3in | inp | pin | pni | avg  |
|-------------|-------------|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|------|
| FB15k       | LOGICE      | 0.50 | 0.65 | 0.70 | 0.52 | 0.33 | 0.56 | 0.58 | 0.71 | 0.55 | 0.58 | 0.67 | 0.70 | 0.58 |
|             | BETA        | 0.44 | 0.51 | 0.50 | 0.60 | 0.52 | 0.58 | 0.48 | 0.56 | 0.53 | 0.33 | 0.43 | 0.59 | 0.70 | 0.58 |
|             | Q2B         | 0.30 | 0.22 | 0.26 | 0.33 | 0.27 | 0.30 | 0.14 | 0.62 | 0.55 | 0.46 | 0.47 | 0.61 | 0.49 | -    |
| FB15k-237   | LOGICE      | 0.65 | 0.67 | 0.72 | 0.61 | 0.51 | 0.57 | 0.60 | 0.69 | 0.54 | 0.62 | 0.61 | 0.67 | 0.62 | -    |
|             | BETA        | 0.61 | 0.58 | 0.58 | 0.64 | 0.64 | 0.54 | 0.49 | 0.58 | 0.50 | 0.41 | 0.49 | 0.60 | 0.63 | -    |
|             | Q2B         | 0.18 | 0.23 | 0.27 | 0.35 | 0.40 | 0.36 | 0.20 | 0.69 | 0.58 | 0.51 | 0.47 | 0.67 | 0.54 | -    |
| NELL995     | LOGICE      | 0.67 | 0.64 | 0.60 | 0.63 | 0.64 | 0.55 | 0.58 | 0.70 | 0.59 | 0.49 | 0.55 | 0.70 | 0.61 | -    |
|             | BETA        | 0.51 | 0.56 | 0.48 | 0.68 | 0.67 | 0.56 | 0.61 | 0.30 | 0.34 | 0.58 | 0.53 | 0.58 | 0.53 | -    |
|             | Q2B         | 0.15 | 0.29 | 0.31 | 0.38 | 0.41 | 0.36 | 0.35 | 0.30 | 0.34 | 0.58 | 0.53 | 0.58 | 0.53 | -    |

### Table 15. Pearson correlation coefficient (higher better) between learned embedding (diff. entropy for LOGICE and BETA, box size for Q2B) and the number of answers of queries.

| Dataset     | Model       | 1p | 2p | 3p | 2i | 3i | pi | ip | 2in | 3in | inp | pin | pni | avg  |
|-------------|-------------|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|------|
| FB15k       | LOGICE      | 0.28 | 0.50 | 0.56 | 0.47 | 0.34 | 0.38 | 0.43 | 0.56 | 0.46 | 0.45 | 0.48 | 0.56 | 0.46 |
|             | BETA        | 0.22 | 0.36 | 0.38 | 0.39 | 0.30 | 0.31 | 0.31 | 0.44 | 0.41 | 0.34 | 0.36 | 0.34 | 0.36 |
|             | Q2B         | 0.08 | 0.22 | 0.26 | 0.29 | 0.23 | 0.25 | 0.13 | -    | -    | -    | -    | -    | -    |
| FB15k-237   | LOGICE      | 0.33 | 0.53 | 0.61 | 0.45 | 0.37 | 0.37 | 0.47 | 0.58 | 0.44 | 0.52 | 0.49 | 0.57 | 0.48 |
|             | BETA        | 0.23 | 0.37 | 0.45 | 0.36 | 0.31 | 0.32 | 0.33 | 0.46 | 0.41 | 0.39 | 0.36 | 0.48 | 0.37 |
|             | Q2B         | 0.02 | 0.19 | 0.26 | 0.37 | 0.40 | 0.34 | 0.20 | -    | -    | -    | -    | -    | -    |
| NELL995     | LOGICE      | 0.43 | 0.53 | 0.53 | 0.53 | 0.49 | 0.46 | 0.45 | 0.66 | 0.54 | 0.46 | 0.55 | 0.63 | 0.52 |
|             | BETA        | 0.24 | 0.40 | 0.43 | 0.40 | 0.39 | 0.40 | 0.40 | 0.52 | 0.51 | 0.26 | 0.35 | 0.46 | 0.40 |
|             | Q2B         | 0.07 | 0.21 | 0.31 | 0.36 | 0.29 | 0.24 | 0.34 | -    | -    | -    | -    | -    | -    |
Table 16. Answer size prediction mean absolute error (%, lower better) with embedding entropy components for LOGICE and BETA_E, and box size components for Q2B.

| Dataset   | Model   | 1p | 2p | 3p | 2i | 3i | pi | ip | 2in | 3in | inp | pin | pni | avg |
|-----------|---------|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|
| FB15k     | LOGICE  | 81.0 | 51.9 | 46.3 | 62.5 | 73.2 | 28.4 | 47.8 | 65.3 | 37.6 | 54.9 |
|          | BETA_E  | 76.4 | 47.9 | 43.3 | 56.6 | 67.1 | 25.0 | 42.6 | 57.9 | 35.9 | 50.3 |
|          | Q2B     | 42.4 | 50.2 | 45.9 | 63.7 | 70.0 | 60.7 | 61.4 | 9.0  | 42.6 | 49.5 |
| FB15k-237 | LOGICE  | 75.8 | 46.0 | 41.8 | 59.6 | 62.5 | 74.3 | 24.3 | 48.0 | 62.2 | 51.4 |
|          | BETA_E  | 78.6 | 41.3 | 30.3 | 59.3 | 71.2 | 21.1 | 39.7 | 60.8 | 33.0 | 48.4 |
|          | Q2B     | 63.6 | 34.6 | 25.0 | 51.5 | 62.4 | 15.1 | 31.0 | 37.6 | 27.3 | 38.7 |
| NELL995  | LOGICE  | 46.1 | 28.6 | 24.8 | 34.8 | 46.5 | 12.0 | 23.7 | 27.7 | 21.1 | 29.5 |
|          | BETA_E  | 45.0 | 26.6 | 23.0 | 32.0 | 44.1 | 11.1 | 22.1 | 25.5 | 20.4 | 27.7 |
|          | Q2B     | 37.7 | 34.9 | 34.3 | 44.3 | 49.4 | 40.8 | 42.3 | 8.7  | 28.2 | 35.8 |
|          | GQE     | 43.1 | 25.3 | 22.3 | 31.3 | 44.6 | 10.2 | 22.3 | 26.6 | 18.0 | 27.1 |
|          | ip      | 46.7 | 24.0 | 18.6 | 32.4 | 45.3 | 10.8 | 20.5 | 23.9 | 19.3 | 26.8 |
|          | 2i      |        |      |      |      |      |      |      |      |      |      |
|          | 3i      |        |      |      |      |      |      |      |      |      |      |
|          | pi      |        |      |      |      |      |      |      |      |      |      |
|          | ip      |        |      |      |      |      |      |      |      |      |      |
|          | 2in     |        |      |      |      |      |      |      |      |      |      |
|          | 3in     |        |      |      |      |      |      |      |      |      |      |
|          | inp     |        |      |      |      |      |      |      |      |      |      |
|          | pin     |        |      |      |      |      |      |      |      |      |      |
|          | pni     |        |      |      |      |      |      |      |      |      |      |

Table 17. Detailed Hits@3 results for all the Query2Box datasets.

| Generalization | 1p | 2p | 3p | 2i | 3i | pi | ip | 2u | up | avg |
|---------------|----|----|----|----|----|----|----|----|----|-----|
| FB15k         | LOGICE | 84.4 | 64.0 | 57.9 | 70.8 | 80.6 | 41.0 | 59.0 | 76.6 | 51.0 | 65.5 |
| EmQL          | 82.9 | 57.3 | 51.9 | 62.5 | 73.0 | 34.1 | 51.5 | 67.2 | 45.5 | 58.4 |
| Q2B           | 98.5 | 96.3 | 91.1 | 91.4 | 88.1 | 87.8 | 89.2 | 88.7 | 91.3 | 91.4 |
| GQE           | 41.5 | 40.4 | 38.6 | 62.9 | 74.5 | 49.8 | 64.8 | 12.6 | 35.8 | 46.8 |
|               | ip   | 55.5 | 26.6 | 23.3 | 34.3 | 48.0 | 13.2 | 21.2 | 36.9 | 16.3 | 30.6 |
|               | 2u   | 41.8 | 23.1 | 20.5 | 31.8 | 45.4 | 8.1  | 18.8 | 20.0 | 13.9 | 24.8 |
| Entailment    | LOGICE | 88.8 | 64.0 | 57.9 | 70.8 | 80.6 | 41.0 | 59.0 | 76.6 | 51.0 | 65.5 |
| EmQL          | 82.9 | 57.3 | 51.9 | 62.5 | 73.0 | 34.1 | 51.5 | 67.2 | 45.5 | 58.4 |
| Q2B           | 98.5 | 96.3 | 91.1 | 91.4 | 88.1 | 87.8 | 89.2 | 88.7 | 91.3 | 91.4 |
| GQE           | 41.5 | 40.4 | 38.6 | 62.9 | 74.5 | 49.8 | 64.8 | 12.6 | 35.8 | 46.8 |
|               | ip   | 55.5 | 26.6 | 23.3 | 34.3 | 48.0 | 13.2 | 21.2 | 36.9 | 16.3 | 30.6 |
|               | 2u   | 41.8 | 23.1 | 20.5 | 31.8 | 45.4 | 8.1  | 18.8 | 20.0 | 13.9 | 24.8 |
| FB15k-237     | LOGICE | 81.5 | 54.2 | 46.0 | 58.1 | 67.1 | 28.5 | 44.0 | 66.6 | 40.8 | 54.1 |
| EmQL          | 73.7 | 46.4 | 38.9 | 49.8 | 61.5 | 22.0 | 37.2 | 54.6 | 35.1 | 46.6 |
| Q2B           | 100.0 | 99.5 | 94.7 | 92.2 | 88.8 | 91.5 | 93.0 | 94.7 | 93.7 | 94.2 |
| GQE           | 68.0 | 39.4 | 32.7 | 48.5 | 65.3 | 16.2 | 32.9 | 61.4 | 28.9 | 43.7 |
|               | ip   | 73.8 | 40.5 | 32.1 | 49.8 | 64.7 | 18.9 | 36.1 | 47.2 | 30.4 | 43.7 |
|               | 2u   | 73.8 | 40.5 | 32.1 | 49.8 | 64.7 | 18.9 | 36.1 | 47.2 | 30.4 | 43.7 |
| NELL995       | LOGICE | 96.2 | 90.7 | 84.1 | 84.1 | 89.5 | 65.2 | 76.0 | 94.7 | 87.1 | 85.3 |
| EmQL          | 94.1 | 86.0 | 78.7 | 80.4 | 87.1 | 53.6 | 68.5 | 89.0 | 81.2 | 80.1 |
| Q2B           | 99.0 | 99.0 | 97.1 | 99.7 | 99.6 | 98.7 | 98.9 | 98.8 | 98.5 | 98.8 |
| GQE           | 72.8 | 58.0 | 55.2 | 45.9 | 57.3 | 24.8 | 34.2 | 59.0 | 40.7 | 49.8 |