Guessing What’s Plausible But Remembering What’s True: Accurate Neural Reasoning for Question-Answering

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Abstract

Neural approaches to natural language processing (NLP) often fail at the logical reasoning needed for deeper language understanding. In particular, neural approaches to reasoning that rely on embedded generalizations of a knowledge base (KB) implicitly model which facts that are plausible, but may not model which facts are true, according to the KB. While generalizing the facts in a KB is useful for KB completion, the inability to distinguish between plausible inferences and logically entailed conclusions can be problematic in settings like KB question answering (KBQA). We propose here a novel KB embedding scheme that supports generalization, but also allows accurate logical reasoning with a KB. Our approach introduces two new mechanisms for KB reasoning: neural retrieval over a set of embedded triples, and “memorization” of highly specific information with a compact sketch structure. Experimentally, this leads to substantial improvements over the state-of-the-art on two KBQA benchmarks.

1 Introduction

1.1 Background and motivation

The neural techniques that dominate current approaches to NLP are unfortunately rather fallible when a language-based task requires logical reasoning. In particular, basic logical reasoning is needed to answer natural-language questions from a knowledge base (KB). However, neural representations of the KB based on KB embeddings (KBE) perform poorly at reasoning accurately with a KB: as KBEs are designed to generalize the contents of a KB, they tend to perform well at predicting which facts are plausible, but perform less well at performing inferences that depend on which facts are actually present in the KB. In words, they are intended to be differentiable approximations of logical reasoners, but the approximations they make can act as noise when training a neural system end-to-end on any task combining language understanding and reasoning.

1.2 Overview of our approach

Reasoning operators. Our novel KBE approach enables accurately following long chains of reasoning, while maintaining KBE’s key advantages of being fast and differentiable. To avoid well-known complexity issues involved in first-order logical reasoning (Cohen et al., 2017), we implement reasoning using compositional, differentiable functions on weighted sets of entities. In addition to (weighted) set intersection, union, and difference, we also implement two operators for relational reasoning: relation following and relational filtering. Relation following (Cohen et al., 2019a) takes a set of entities \( X \) and a set of relations \( R \) and computes the set of entities related to something in \( X \) via some relation in \( R \):

\[
X._{\text{follow}}(R) \equiv \{ y | \exists r \in R, x \in X : r(x, y) \}
\]

(Here “\( r(x, y) \)” indicates that this triple is in the KB—other notation is listed in Appendix A.) For example, to look up the headquarters of the Apple company one might compute \( Y = X._{\text{follow}}(R) \) where \( X \) and \( R \) are singleton sets containing “AppleInc” and “headquarters of” respectively. Relational filtering removes from \( X \) those entities that are not related to something in set \( Y \) via some relation in \( R \):

\[
X._{\text{filter}}(R, Y) \equiv \{ x \in X | \exists r \in R, y \in Y : r(x, y) \}
\]

For example, \( W._{\text{filter}}(R, Y) \) would find the companies in \( W \) with headquarters in Cupertino, if \( R \) and \( Y \) are as in the previous example.

This group of operators is richer than those supported by prior KBE approaches to reasoning (see § 2). We also extend KBE to allow more
accurate differentiable reasoning, by supplementing geometric operations in embedding space with two new mechanisms: triple retrieval and sparse-dense encodings.

**Triple retrieval.** We use maximal inner-product search (MIPS) to implement neural retrieval over KB triples—i.e., our system is a hybrid of conventional KBE and memory networks (Weston et al., 2014). For example, consider computing $y \in \{x\} . \text{follow}(\{r\})$. The TransE KBE method (Bordes et al., 2013) estimates the embedding for $y$ with differentiable functions of $e_x$ and $e_r$. Our method instead approximates $e_y$ as a function of $e_x$, $e_r$, and a memory that includes embeddings of every KB triple. Using the full KB, instead of a dense approximation of it, allows more accurate reasoning, but we also show that this approach can be efficient.

**Sparse-dense encodings.** Our formulation of logical reasoning requires manipulating sets of entities. Prior KBE approaches for modeling sets encoded sets as parametric functions on embedding space, such as Gaussians (Vilnis and McCallum, 2014) or rectangles (Vilnis et al., 2018). These parametric functions were carefully designed to balance expressiveness with efficiency, but are typically unable to represent accurately the very specific sets required in KB reasoning. Encode a specific sets of interest, we treat these parametric set representations as “candidate generators”, and use a sparse randomized data structure called a count-min sketch (Cormode and Muthukrishnan, 2005; Daniely et al., 2016) to store the degree of membership of candidate entities. We show that this combination leads to a set representation which is differentiable, compact, and highly accurate, even if the parametrically-defined generators only loosely approximate the sets of interest.

### 1.3 Contributions

To summarize, our main contribution is efficient neural implementation of an expressive group of set and relational operators, allowing accurate compositional reasoning over sets of embeddings. Unlike previous KBE approaches, our system enjoys all of the following properties (see § 4): (1) closure under composition, that is, the output of any operator can be used as an input to any other operator, making long reasoning chains possible; and (2) accuracy relative to the original KB, in addition to supporting plausible reasoning based on geometric areas of embedding space.

Additionally, in § 3.3, we show that (3) embeddings learned by external pre-training methods such as BERT (Devlin et al., 2018) can be adapted to support reasoning with our method; and that the approach is efficient for large KBs.

## 2 Related work

**KBE and reasoning.** There are many KBE methods, surveyed in (Wang et al., 2017). Most support only a few of the set operations discussed above, and usually those operations can only be composed in limited ways.

In more detail, all KBE methods generalize a KB by learning a model that scores the plausibility of a potential KB triple $r(x, y)$. Many KBE models also support relation following, at least for singleton sets. However, most KBE methods give poor results when relation-following operations are composed (Guu et al., 2015), as in computing $x . \text{follow}(r_1) . \text{follow}(r_2)$. To address this, some KBE systems learn to follow a path, or chain of relations (Guu et al., 2015; Lin et al., 2015; Das et al., 2016). Very few KBE schemes have considered compositionality beyond path-following: one notable exception is the graph-query embedding (GQE) method, which supports compositions of relation-following and set intersection (Hamilton et al., 2018). Our method extends GQE and related approaches: as well as allowing composition of relation following operations and set intersection, we support set union and relation filtering. Additionally we present formal bounds on the accuracy of reasoning using our embedding scheme—bounds obtainable due to the addition of triple retrieval and the sparse-dense set encoding scheme.

Another connection between KBE and reasoning is illustrated by (Demeester et al., 2016; Rastogi et al., 2017), in which relational constraints such as transitivity or implication are incorporated into a KBE model. Here we focus on a different goal, i.e., seeking to maximize performance on compositional queries in the absence of prior knowledge in the form of constraints.

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1Specifically, TransE uses the estimate $e_y = e_x + e_r$, where $e_x$, $e_y$, and $e_r$ are the embeddings for $x$, $y$, and $r$ respectively. Other KBE methods approximate $e_y$ with different functions of $e$ and some embedded representation of $r$.

2E.g., as noted above, translational embedding schemes like TransE (Bordes et al., 2013) which estimate the embedding for $y$ as $e_y = e_x + e_r$, where $e_x$, $e_r$, and other methods (Guu et al., 2015; Liu et al., 2017) use the estimate $e_y = e_xM_r$, where $M_r$ is a matrix representing $r$. 

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Dense neural representations of sets. Another line of prior work has looked at representing sets of entities with embeddings (Vilnis and McCallum, 2014; Vilnis et al., 2018; Zaheer et al., 2017). Relative to prior work, our representation has the advantage of being closed under all of intersection, union, relation following, and relational filtering. Although most prior work has not explicitly considered compositional-ity of set operations, box embeddings (Vilnis et al., 2018) are closed under intersection, and quantum logic (Svozil, 1998) is closed under intersection and negation, and approximately closed under union (via computation of an upper bound on the union set.) It is also known that any intersection of hyperplanes is a convex set (Barber et al., 1996).

Sparse neural representations of sets. One simple way to represent sets is with “k-hot” vectors. Assume a universe $U$ which is a set of integers “object ids” $\{1, \ldots, N\}$. Then the $k$-hot vector representation of a set $A \subseteq U$ is the vector $v_A \in \mathbb{R}^N$ such that $v_A[i] = 1$ if $i \in A$ and 0 otherwise. Such vectors can also encode weighted sets by allowing $v_A[i]$ to be a real number, and $k$-hot vectors can be easily combined compositionally: if vectors $v_A$ and $v_B$ represent sets $A$ and $B$, then $v_A + v_B$ represents $A \cup B$ and $v_A \odot v_B$ represents $A \cap B$. For $k$-hot vectors, relation following can be implemented as matrix multiplication, and relational filtering can be implemented in terms of relation following and intersection (Cohen et al., 2019a). However, such “localist” representations have an important disadvantage: because sets encode entity ids, not embeddings, it is difficult for learned neural modules to produce these sets.\footnote{Also, for a large KB, the dimension of $k$-hot vectors is large, making them inefficient if the usual GPU-friendly representation of tensors is used. While in some cases sparse-matrix encodings can be used to speed up computation and reduce storage, sparse tensor operations are still only partly supported in many deep-learning frameworks.}

Our set representation supports the same operators as $k$-hot vectors, but because sets representations are based on embeddings, not entity ids, it is much easier for neural modules to learn to produce set expressions for our scheme. This leads to much better performance on benchmark tasks, as shown below.\footnote{Further, while we do make use of sparse, randomized structures, the sparsity is much more limited (see § 4), so no special sparse-matrix support is needed to implement our methods.}

Key-value memory networks. Our triple retrieval mechanism is a type of key-value mem-

ory network (Miller et al., 2016b), and since the mechanisms we use for intersection and union are quite simple, this work could also be described as augmenting a key-value memory network with a sparse-dense component. To our knowledge this is novel, and ablation experiments in § 5 show that it greatly improves performance. This paper also contributes to the formal understanding of the expressive power of key-value memory networks: while they can be trained to implement chains of relation-following operations over singleton sets, to our knowledge there has been no prior analysis of when, or whether, they can implement more complex relational set-based operations.

3 Compositional reasoning over sets

We now describe EmQL (for Embedding Query Language), our neural set representation, and the corresponding approximations of set and relational operators. We assume here that all the sets represented are subsets of a fixed universe $U$ of cardinality $N$, and identify the $i$th element of $U$ with $i$ where convenient. Additional notation used here is given in Appendix A.

3.1 Encoding and decoding sets

Background. A baseline representation for a weighted set $X \subseteq U$ is a $k$-hot vector $v_X \in \mathbb{R}^N$, where $v_X[i]$ holds the non-negative real weight of element $i$ in $X$. We assume that each entity $i$ has an embedding $e_i \in \mathbb{R}^d$; $E \in \mathbb{R}^{d \times N}$ is the matrix of all embeddings.

Encoding sets. We represent a set $X$ with a pair $(a_X, b_X)$. $a_X = \sum_{i} v_X[i] e_i$, $b_X = S_H(v_X)$. The centroid $a_X$ identifies the general region containing elements of $X$ and $b_X$ is a count-min sketch of the elements of $X$ (Cormode and Muthukrishnan, 2005). Appendix B summarizes the technical details of count-min sketches—briefly, a count-min sketch supports a differentiable operator $CM(i, b_X)$ that returns, with high probability, the weight $v_X[i]$ for entity $i \in X$. The data for the sketch $b_X$ is an $N_D \times N_W$ matrix, where $N_W$ and $N_D$ are called the width and depth of the sketch. We use fixed values for the hyperparameters $N_W$ and $N_D$ for all sets $X$ in our experiments.

Because the sketch $b_X$ will produce incorrect values with some probability, it is important not to query the sketch too many times. The set of candidates for querying the sketch is a sphere centered on $a_X$. This sphere can be viewed as a soft type for the entities in $X$, intended to encode general properties of $X$’s elements, for example “US mid-size
cities,” or “Ph.D. students in NLP”. In our set operators, sketches are only queried for entities of the correct soft type, making it possible to use much smaller sketches (see § 4).

Hard types. Sometimes there is a known “hard” partitioning of entities, for instance the disjoint “film” and “person” types in a film KB. Hard types can be implemented by encoding a type in some subset of the embedding dimensions, and giving these dimensions large magnitude to push entities of disjoint hard types far apart, as detailed in Appendix C.3.

Sketchless sets. When a neural function is used to compute a set representation \( Y \), it is often useful to couple a predicted centroid \( a_Y \) with the vacuous, always true sketch, such that \( CM(i, b_Y) = 1 \forall i \in U \); the count-min sketch \( b_Y \) will be an all-ones matrix of the correct size. The advantage of this is that it can be difficult to predict \( b_Y \), which is an id-based representation; however, once specific entities are identified in KB reasoning, sketches make it possible to propagate information through KB operations without losing much information.

Decoding a set. To reconstruct the original set from its encoding, we take the \( k \) elements with highest dot product \( a_Y^T e_i \), where \( k \) is a fixed hyperparameter. This is done efficiently with a maximum inner product search (MIPS), which we write \( \text{TOP}_k(a_X, E) \). These top \( k \) elements are then filtered by the count-min sketch, resulting in a sparse (no more than \( k \) non-zeros) decoding of the set representation

\[
\hat{v}_X[i] = \begin{cases} 
CM(i, b_X) \cdot \text{softmax}(a_Y^T e_i) & \text{if } i \in \text{TOP}_k(a_X, E) \\
0 & \text{else} 
\end{cases} 
\]  

(1)

3.2 Set operations

Intersection and union. Set intersection and union of sets \( A \) and \( B \) are computed as sparse-dense representations \( (a_{A \cap B}, b_{A \cap B}) \) and \( (a_{A \cup B}, b_{A \cup B}) \), respectively. Both for intersection, the dense soft types are only informative if the soft types of \( A \) and \( B \) are similar:

\[
a_{X \cap Y} = a_{X \cup Y} = \frac{1}{2}(a_X + a_Y)
\]

For the sketches, we exploit the property (see Appendix B) that if \( b_A \) and \( b_B \) are sketches for \( A \) and \( B \) respectively, then a sketch for \( A \cup B \) is

\[
b_A + b_B, \text{ and the sketch for } A \cap B \text{ is } b_A \odot b_B \text{ (where } \odot \text{ is Hadamard product), so:}
\]

\[
b_{X \cap Y} = b_X \odot b_Y
\]

\[
b_{X \cup Y} = b_X + b_Y
\]

Relation following. Relation following relies on an embedding matrix \( K \) for KB triples that parallels the element embedding matrix \( E \): for every triple \( t = (r, x, y) \) in the KB, \( K \) contains a row \( r_t = [e_r; e_x; e_y] \) concatenating the embeddings for \( r, x, \) and \( y \). The procedure to compute \( Y = X . follow(R) \) is analogous to set decoding.

First we create a query \( q_{R,X} = [\lambda \cdot a_R; a_X; 0] \) by concatenating the centroids for \( R \) and \( X \) and padding it to the same dimension as triple embeddings. \( \lambda \) is a hyper-parameter scaling the weight of the relation part. Next using the query \( q_{R,X} \), we perform a MIPS against all triples in KB \( K \) to get the top \( k \) triples matching this query, and these triples are filtered with the sketches of \( X \) and \( R \). Let \( r_t = [e_{r_t}; e_{x_t}; e_{y_t}] \) be the representation of triple \( t = (x_t, y_t) \). Its score is

\[
s(r_t) = CM(i, b_R) \cdot CM(j, b_X) \cdot \text{softmax}(q_{R,X}^T r_t)
\]

We can then project out the objects from the top \( k \) triples as a sparse \( k \)-hot vector:

\[
\hat{v}_Y(\ell) = \sum_{r_t \in \text{TOP}_k(q_{R,X}, K), t = (\ell, y_t)} s(r_t)
\]

Finally \( \hat{v}_Y \) is converted to a set representation \( (a_Y, b_Y) \), which represents the output of the operation, \( Y = X . follow(R) \).

Relational filtering. For \( X . \text{filter}(R, Y) \), the query must also be aware of the objects of the triples, since they should be in the set \( Y \). The query vector is thus \( q_{R,X,Y} = [\lambda \cdot a_R; a_X; a_Y] \). Again, we perform a retrieval using query \( q_{R,X,Y} \), but we filter with subject, relation, and object sketches \( b_R, b_X, b_Y \), so the score of an encoded triple \( r_t \) is

\[
s(r_t) = CM(i, b_R) \cdot CM(j, b_X) \cdot CM(\ell, b_Y) \cdot \text{softmax}(q_{R,X,Y}^T r_t)
\]

The same aggregation strategy is used as for the follow operation, except that scores are aggregated over the subject entities instead of objects.

3.3 Using pre-trained embeddings

In § 5.1 we describe how embeddings can be trained to best support reasoning. It is also useful
to have entity embeddings that are easy to predict from language. To encourage this, we can make the trained embeddings for entities and relations be based on language-based pre-training.

As one implementation of this idea, we extended EmQL as follows. Let $e_x^0$ be the embedding of the [CLS] token from a BERT (Devlin et al., 2018) encoding of the canonical name for entity $x$, and let $e_x^1$ be a vector unique to $x$. Our pre-trained embedding for $x$ is then $e_x = [W^T e_x^0; e_x^1]$, where $W$ is a learned projection matrix. The embedding of relation $r$ is set to the BERT encoding ([CLS] token) of the canonical name of relation $r$.

In our experiments, $e_x^1$ was indispensable, since using only a single projection matrix $W$ and pre-trained BERT embeddings did not converge to useful embeddings. An alternative for further work would be to fine-tune BERT for reasoning.

### 3.4 Training the embeddings

All the representations and operations defined above are approximations. While the sketches prevent an element $x' \not\in X$ from getting a high score, the use of the top-$k$ operator to retrieve candidates means that set decoding only has high recall if the elements in $X$ are close enough in the inner product space that they can be recovered with the top-$k$ query. To alleviate this, we need to train the entity and relation embeddings to minimize the mismatch between sparse-dense and explicit set representations. Specifically, let $(a_X, b_X)$ be the sparse-dense representation of set $X$ and $v_X$ the corresponding $k$-hot decoding. We minimize

$$\text{cross_entropy}(\text{softmax}(a_X^T, E), v_X / |v_X|_1)$$

Note that this objective ignores the sketch, so it forces the dense representation to do the best job possible on its own. Note that here $X$ can be the result of a computation, such as the output of some chain of set operations, as explained in more detail in § 5.1.

### 4 Analysis

**Closure properties and accuracy.** By construction, our operations are closed under composition because they all take and return the same sparse-dense representations. However, closure would be of no use if accuracy could not be maintained.

Fortunately, EmQL’s sparse-dense representation can do well even if the dense $k$-nearest neighbor retrieval is in itself imprecise. More specifically, consider a set $A$ with $|A| = m$ and sparse-dense representation $(a_A, b_A)$. Suppose that $k = cm$ ensures that all $m$ elements of $A$ are retrieved as $k$-nearest neighbors of $a_A$; in other words, retrieval precision may be as low as $1/c$. By Theorem 2 in Appendix B, a sketch of size $2m \log_2 \frac{m}{\delta}$ will recover all the weights in $A$ with probability at least $1 − \delta$. Thus, a sketch of size $\sim 4k$ would fully recover a set of size 100 with 99% probability even if retrieval precision was just 10%.

Note that this does not immediately imply the correctness of the operations in § 3, since they are not guaranteed to produce the true centroid of the sets being represented; nor, of course, does it guarantee that retrieval precision can be ensured in training. Hence performance must still be verified experimentally. However it does strongly suggest that relatively small sketches will be sufficient for accuracy, even if top-$k$ queries have low precision. Furthermore, this is independent of KB size—which, combined with the existence of approximate sublinear top-$k$ methods, suggests that our approach can potentially scale to very large KBs.

**Size of sketches.** In our experiments we limit our training by assuming sets are of size $m < 100$, and that $c = 10$. Using 32 numbers per potential set member leads to $\delta \approx \frac{1}{10}$. Put another way, sets of 100 elements require about as much storage as the BERT contextual encoding of 4 tokens, and the sketch for 100 elements also requires about 1/4 the size of storing 100 embeddings with $d = 128$.

It is also easy to see that for a set of size $m$, close to half of the numbers in the sketch will have non-zero values. Thus only a moderate savings in space is obtained by using a sparse-matrix data structure: it is quite practical to encode sketches with GPU-friendly dense tensor data structures.

### 5 Experiments

We evaluate EmQL first intrinsically for its ability to model set expressions (Hamilton et al., 2018), and then extrinsically as the reasoning component in two multi-hop KB question answering benchmarks (KBQA).

#### 5.1 Learning to reason with a KB

We experimented with the KB provided by the WikiMovies dataset (Miller et al., 2016a), also

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6 In addition, a certain level of retrieval precision is not sufficient in relation following or filtering because of the additional subject or object constraints on the retrieved triples.  
7 Of course, directly storing 100 embeddings is less useful for modeling, since that representation does not support operations like relation following or intersection.  
8 Each row will have had $m$ values hashed into it, so if there were no collisions then $m$ values will be non-zero.
used in MetaQA (Zhang et al., 2018). The WikiMovies KB includes facts about movies and (after adding inverse relations) contains \(\sim\)43k entities, 18 relations and \(\sim\)393k triples.

To generate set expressions, we first compute all sets of the form \(\{x\}.follow(\{r\})\), that is, sets that can be obtained by following a single entity and relation, such as all movies directed by Christopher Nolan. We call these basic sets. We generated 39,524 non-singleton basic sets from the KB. For intersection and union, we generated all pairs of non-disjoint basic sets \(A\) and \(B\), giving 67,728 pairs of sets.9 For relation following, we use for the input set \(X\) a basic set of entities that share some common tail of the same relation \(r\), and use \(R = \{r\}\). (For example, we might generate an example from the set of movies that star Robert Downey Jr., with basic set input \(X = \{\text{Iron Man}, \text{Avengers}, \ldots\}\) and the relation \(r = \text{stars}_\text{actor}\). The desired output \(Y = X.\text{follow}(r)\) for this example is the set of actors that co-starred with Robert Downey Jr.) We generate 52,364 examples for relation following.10

We trained our model on 4 different tasks: set representation (encoding and decoding a set), intersection, union, and relation following. We randomly sample 80% of the data for each task as training data and keep the remaining 20% as test. At training time, each mini-batch contains examples for each task, evenly distributed. The final loss is the unweighted loss over all tasks. We used a count-min sketch with \(N_D = 30\) and \(N_W = 2000\), and embedding dimension \(d = 64\).

The results are shown in Table 1. We measured the precision, recall and F1 of the top \(k\) values in each computed set (averaged across the test cases). The sketches ensure that sets are high precision (for this sketch size, precision is always 99% or better), but the experiments verify that training can make the sets coherent, so relatively small \(k\) can be used while still obtaining good recall.

On Table 2 we show performance with a sketch one-tenth the size (with \(N_W = 200\)) and an ablated model with no sketch. The results show that sketches are essential for obtaining high precision. This is true especially for larger sets, but even for \(k = 10\), substantial gains in precision are obtained by the addition of sketches.

| Set | k=1 | k=10 | k=100 | k=1000 |
|-----|-----|------|-------|--------|
| R   | 94.7 | 98.9 | 99.8  |         |
| P   | 100.0 | 100.0 |       |         |
| F1  | 96.5 | 99.2 | 99.9  |         |

| Intersect | k=1 | k=10 | k=100 | k=1000 |
|-----------|-----|------|-------|--------|
| k=100     | 91.7 | 97.7 | 99.7  |         |
| R         | 71.0 |     |       |         |
| P         | 99.8 | 99.4 | 99.2  | 98.9   |
| F1        | 74.7 | 92.7 | 98.8  | 99.3   |

| Union     | k=1 | k=10 | k=100 | k=1000 |
|-----------|-----|------|-------|--------|
| k=100     | 93.0 | 98.8 |       |         |
| R         | 99.5 | 99.6 | 99.7  | 99.8   |
| P         | 100.0 | 99.7 | 99.2  | 98.8   |
| F1        | 16.1 | 47.0 | 65.8  | 84.3   |

| Follow    | k=1 | k=10 | k=100 | k=1000 |
|-----------|-----|------|-------|--------|
| k=100     | 93.0 | 94.9 |       |         |
| R         | 10.3 | 52.1 | 81.7  | 93.0   |
| P         | 100.0 | 100.0 |       | 100.0  |
| F1        | 16.4 | 59.2 | 84.7  | 94.9   |

Table 1: Precision, recall and F1 for model jointly trained on all four reasoning tasks.

Table 3: Recall of set-follow operation with various count-min sketches.

| recall (single task) | k=1 | k=10 | k=100 | k=1000 |
|----------------------|-----|------|-------|--------|
| 9.7                  | 49.2 | 78.1 | 91.8  |        |
| recall (multi task)  | 13.3 | 28.1 | 81.7  | 93.0   |
| max recall           | 13.3 | 28.1 | 81.7  | 94.1   |

Table 2: Precision of retrieval for the set-follow operation with various count-min sketches.

Finally, Table 3 shows recall for relation following operations when trained jointly, compared to an ablated system that trains only on relation following. We also report here the maximum recall obtainable by retrieving \(k\) results. Joint training improves performance at all values of \(k\), and brings performance close to the theoretical optimum. The benefits of joint training are most likely due to the fact that the requirement of coherency for embeddings is shared by all operations.11

5.2 Question answering

To evaluate the reasoning operations as a neural component in a larger system, we experimented with two KBQA datasets, MetaQA (Zhang et al., 2018) and WebQuestionsSP (Yih et al., 2015). The input to the QA system will be a question \(q\) in natural language and a set of entities \(X_q\) mentioned in the question, and the output is a set of answers \(Y\). In training only the answers are available—no information is given about the latent logical query that should be used to produce the answers. For each task, set operations were pre-trained (as in § 5.1) and then the KB embeddings were fixed while training the QA model.

9Although unions could be computed over non-overlapping sets, we believe that it is most common to union together sets of similar types, and that this heuristic produces more reasonable examples.

10One basic set can share multiple properties, so can give rise to multiple examples of relation following.

11Note that while the tasks are different they involve the same group of basic sets, which must be coherent whenever they appear. In particular, a basic set used in the test data for one task could appear in the training data for another. We assume oracle question entities \(X_q\) is provided.
5.2.1 Datasets and models

MetaQA. The MetaQA dataset (Zhang et al., 2018) contains multi-hop questions in the movie domain, which can be answered using the KB described in § 5.1. The dataset contains 300k 2-hop and 300k 3-hop questions. An examples of a 2-hop question is “When were the movies directed by Christopher Nolan released?” To answer such questions, the model should find the movies directed by Christopher Nolan, such as Inception, and then find the years that those movies were released. Following prior work, we assume the number of hops is known. The model\(^\text{13}\) for MetaQA’s 2-hop questions is

\[
\hat{Y} = X_q, \text{follow}(R_1), \text{follow}(R_2) - X_q
\]

\[
R_1 = (a_1, b_1), \quad a_1 = W_1^T \text{encode}(q)
\]

\[
R_2 = (a_2, b_1), \quad a_2 = W_2^T \text{encode}(q)
\]

where \(W_1\) and \(W_2\) are learned parameters, \(b_1\) is a vacuous sketch, and \(\text{encode}(q)\) is obtained by pooling the (non-contextual) embeddings of words in \(q\) (see Appendix C.2).

This model is as simple as it is because all the machinery needed to reason with the KB is encapsulated in the follow operation of § 3. All the model now needs to predict is which relations to use in the inference chain from the questions. In this model, the predicted centroid of each relation is defined by a projection from an embedding of the question, and this is coupled with a vacuous sketch. The model for the 3-hop case is analogous.

WebQuestionsSP. This dataset (Yih et al., 2015) contains 4,737 natural language questions generated from Freebase. Questions in WebQuestionsSP are a mixture of 1-hop and 2-hop questions, sometimes followed by a relational filtering operation. The intermediate entities of 2-hop questions are of “Compound Value Type” (CVT) entities—entities that do not have names, but describe \(n\)-ary relationships between entities. For example, answering the question “Who is Barack Obama’s wife?” might require using the triples \(\text{has_marrige(Barack_Obama, cvt1)}\) and \(\text{spouse(cvt1, Michelle_Obama)}\) where the CVT entity \(\text{cvt1}\) represents a marriage relationship for a couple—and the same CVT entity might have other properties in the KB such as \(\text{start\_since(cvt1, 1992)}\). Since there is no \(\text{wife\_rel}\) relation, but only

\(^{13}\)Here \(A - B\) is the set difference operator, and it used because questions like ‘what other movies were directed by the director of Inception?’ exclude the entities in \(X_q\). Please refer to Appendix C.2 for details.

| Datasets and Models          | Train | Dev  | Test  |
|------------------------------|-------|------|-------|
| MetaQA 2-hop                 | 118,980 | 14,872 | 14,872 |
| MetaQA 3-hop                 | 114,196 | 14,274 | 14,274 |
| WebQuestionsSP               | 2,848  | 250  | 1,639 |

(a) Number of train/dev/test data

| Datasets and Models          | Triples | Entities | Relations |
|------------------------------|---------|----------|-----------|
| MetaQA                       | 392,906 | 43,230   | 1,639     |
| WebQuestionsSP               | 1,352,735 | 904,938 | 695       |

(b) Size of KB

Table 4: Statistics of datasets

A \(\text{spouse}\) relation, the QA system must filter the output of the chain of follow operations by a test for female gender. Thus the logical inference needed for this question might be written \(X_q, \text{follow}(R_1), \text{follow}(R_2), \text{filter}(R_3, Z)\), where \(R_1\), \(R_2\), and \(R_3\) are the relations \(\text{has\_marriage, spouse, and gender}\), and \(Z\) is set \{female\}.

The model we use is similar to the model for MetaQA, except that the final stage is a union of several submodels—namely, chains of one and two follow operations, with or without relational filtering. As above, the sets that are predicted from the query \((R_1, R_2, R_3)\) are centroid queries projected from question encoding coupled with vacuous sketches. The superscripts \(e\) or \(cvt\) indicate a hard type for the relations (see Appendix C.3 for more details).

\[
X_1 = X_q, \text{follow}(R_1^{e})
\]

\[
X_2 = X_q, \text{follow}(R_1^{cvt}), \text{follow}(R_2^{e})
\]

\[
\hat{Y} = X_1 \cup X_2 \cup (X_1 \cup X_2), \text{filter}(R_3, Z)
\]

Prediction of the relations is similar to the MetaQA model, but we used a BERT (Devlin et al., 2018) encoding of the question. The learned embeddings are also adaptations of BERT embeddings of entity and relation names (see § 3.3).

We used a subset of Freebase obtained by gathering triples that are within 2-hops of the topic entities in Freebase. We exclude a few extremely common entities and restrict our KB subset so there are at most 100 tail entities for each subject/relation pair (reflecting the limitation of our model to sets of cardinality less than 100). The statistics of both KBs are listed in Table 4.

5.2.2 Baselines

We compare with these baselines. Key Value Memory Network (KV-Mem) (Miller et al., 2016a) and ReifKB (Cohen et al., 2019b) are end-to-end systems for multi-hop inference on KBs. ReifKB is similar to our method but uses a localist encoding based on \(k\)-hot vectors and sparse matrices to encode relations. GRAFFT-Net (Sun et al., 2018) runs a Graph-CNN based
model on a small subset of KB retrieved with some heuristics. PullNet (Sun et al., 2019) learns like GRAFT-Net but iteratively retrieves facts from a KB. Intermediate training signals are required to train PullNet.

### 5.2.3 Results

The results are shown on Table 5. We achieved a new state-of-the-art on the MetaQA 3-hop and WebQuestionsSP datasets, beating the previous state-of-the-art by a large margin (7.7% and 5.8% hits@1 absolute improvement). The results on the MetaQA 2-hop dataset are comparable to the previous state-of-the-art. We note that unlike PullNet, EmQL does not require any intermediate supervision—it learns only from the final answers.

We also consider two ablated versions of our model EmQL (no-sketch) and EmQL(no-constr). EmQL (no-sketch) uses only a centroid embedding. It works consistently worse than the full model for all datasets. This emphasizes the value of including an accurate reasoning model as a neural component in KBQA, which were also not used in the ReifKB baseline—so it is very similar to the ReifKB model. The main difference is that for EmQL (no-constr), predicted relations are a direction in embedding space, rather than a k-hot vector. This leads to 12.5% point improvement in performance over ReifKB on WebQuestionsSP. See Appendix D.2 for more ablated results.

An alternative to adding sketches would be increasing the dimension of entity embeddings. We also experimented with EmQL (no-sketch) on MetaQA by increasing the embedding dimension $d$ until GPU memory was exceeded. Table 6 shows that even with embeddings sizes 8 times larger, the model without a count-min sketch still performs much worse on the downstream QA task.

| KB embeddings and the QA model, using just the QA data. The results are shown on Table 7a and Table 7b. Pre-training the KB embeddings (fix-kge) consistently outperforms jointly training KB embeddings for the QA model (joint). In this experiment, we also varied $k$, the top-$k$ entities retrieved at each step. We also observed that for large $k$ on the MetaQA task, jointly training KB embeddings and the QA model appears to be prone to overfitting. |

| k  | 10  | 20  | 50  | 100 | 200 |
|----|-----|-----|-----|-----|-----|
| EmQL(joint) | 78.7 | 80.1 | 89.7 | 95.2 | 89.4 |
| EmQL(fix-kbe) | 94.7 | 96.5 | 98.8 | 99.1 | 99.2 |

### Table 6: Hits@1 on MetaQA-3hop, varying $d$ for embedded entities.

| $d$ | 64  | 128 | 256 | 512 | 1024 |
|-----|-----|-----|-----|-----|-----|
| EmQL (no sketch) | 60.9 | 61.8 | 62.5 | 65.3 | OOM |

In another experiment, we jointly trained the

| Table 7: Hits@1 (joint v.s. fix-kbe) varying $k$ for top $k$ retrieval. |

| k  | 100 | 200 | 500 | 1000 | 2000 |
|----|-----|-----|-----|------|------|
| EmQL(joint) | 44.9 | 57.0 | 63.4 | 65.7 | 66.6 |
| EmQL(fix-kbe) | 52.7 | 61.5 | 72.2 | 75.5 | 76.2 |

### 6 Conclusions

KBE methods are designed to be differentiable approximations of logical reasoners: they perform well at predicting which facts are plausible, but less well at performing inferences that depend on facts being actually present in the KB. Hence the approximate reasoning performed by KBE methods introduce noise when training a neural system end-to-end on any task combining language understanding and reasoning. Here we implement more accurate KB reasoning with an expressive group of compositional, differentiable functions on weighted sets of entities. To do this we extend prior KBE methods with two new constructs: triple retrieval, using fast top-$k$ retrieval from a KB of embedded triples; and sparse-dense encodings, which combine a count-min sketch for entity weights with a centroid in embedding space. Under reasonable assumptions, this allows provably accurate representations with sketches containing a few dozen numbers per set element. Our method can be trained to have very high precision and high (more than 80%) recall for individual reasoning steps. These individual steps can also be accurately composed.

We also show that embedding a pre-trained reasoner into two KBQA systems gives strong experimental results on two tasks involving compositional reasoning. For MetaQA, we obtain a new state-of-the-art of 99.1 hits@1 on 3-hop questions, more than 7 points higher than the previous best result. For WebQuestionsSP, we obtain a new
state-of-the-art of 75.5 hits@1, more than 5 points higher than the previous best score. Ablation studies show that the sparse-dense representation is important, and that it significantly outperforms even very large dense-only embeddings.

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A Notation

The notation used in this paper is summarized in Table 8.

B Background on count-min sketches

B.1 Definitions

Count-min sketches (Cormode and Muthukrishnan, 2005) are a widely used randomized data structure. We include this discussion for completeness, and our analysis largely follows (Daniely et al., 2016).

A count-min sketch, as used here, is an approximation of a vector representation of a weighted set, as outlined in § 2. Assume a universe \( U \) which is a set of integer “object ids” from \( \{1, \ldots, N\} \). A set \( A \subseteq U \) can be encoded as a vector \( \mathbf{v}_A \in \mathbb{R}^n \) such that \( \mathbf{v}_A[i] = 0 \) if \( i \notin S \), and otherwise \( \mathbf{v}_A[i] \) is a real-numbered weight for entity \( i \) in set \( S \). The purpose of the count-min sketch is to approximate \( \mathbf{v}_A \) with limited storage.

Let \( h \) be a hash function mapping \( \{1, \ldots, N\} \) to a smaller range of integers \( \{1, \ldots, N_W\} \), where \( N_W \ll N \). The primitive sketch of \( \mathbf{v}_A \) under \( h \), written \( \mathbf{s}_h(\mathbf{v}_A) \), is a vector such that

\[
\mathbf{s}_h(\mathbf{v}_A)[j] = \sum_{i; h(i) = j} \mathbf{v}_A[i]
\]

Algorithmically, this vector could be formed by starting with an all-zero’s vector of length \( N_W \), then looping over every pair \((i, w_i)\) where \( w_i = \mathbf{v}_A[i] \) and incrementing each \( \mathbf{s}_h[j] \) by \( w_i \). Examining this algorithm, it is clear that these primitive sketches have the following property: for any two sets \( A \) and \( B \),

\[
\mathbf{s}_h(\mathbf{v}_A + \mathbf{v}_B) = \mathbf{s}_h(\mathbf{v}_A) + \mathbf{s}_h(\mathbf{v}_B)
\]

It is also easy to show that

\[
\mathbf{s}_h(\mathbf{v}_A \odot \mathbf{v}_B) = \mathbf{s}_h(\mathbf{v}_A) \odot \mathbf{s}_h(\mathbf{v}_B)
\]

A primitive sketch \( \mathbf{s}_h \) contains some information about \( \mathbf{v}_A \): to look up the value \( \mathbf{v}_A[i] \), we could look up \( \mathbf{s}_h[h(i)] \), and this will have the correct value if no other set element \( i' \) hashed to the same location. We can improve this by using multiple hash functions.

A count-min sketch is a matrix where each row is a primitive sketch constructed with a different hash function. Specifically, let \( H = \{h_1, \ldots, h_{N_D}\} \) be a list of \( N_D \) hash functions mapping \( \{1, \ldots, N\} \) to the smaller range of integers \( \{1, \ldots, N_W\} \). The count-min sketch \( \mathbf{S}_H(\mathbf{v}_A) \) for a \( \mathbf{v}_A \) under \( H \) is a matrix such that each row \( j \) is the primitive sketch of \( \mathbf{v}_A \) under \( h_j \). This sketch is an \( N_W \times N_D \) matrix: \( N_W \) is called the sketch width and \( N_D \) is called the sketch depth.

Let \( \mathbf{S} \) be the count-min sketch for \( A \). To “look up” (approximately recover) the value of \( \mathbf{v}_A[i] \), we compute this quantity

\[
CM(i, \mathbf{S}) \equiv \min_{j=1}^{N_D} \mathbf{S}[j, h_j(i)]
\]

In other words, we look up the hashed value associated with \( i \) in each of the \( N_D \) primitive sketches, and take the minimum value.

B.2 Linearity and implementation nodes

Count-min sketches also have a useful “linearity” property, inherited from primitive sketches. It is easy to show that for any two sets \( A \) and \( B \) represented by vectors \( \mathbf{v}_A \) and \( \mathbf{v}_B \)

\[
\begin{align*}
\mathbf{S}_H(\mathbf{v}_A + \mathbf{v}_B) &= \mathbf{S}_H(\mathbf{v}_A) + \mathbf{S}_H(\mathbf{v}_B) \\
\mathbf{S}_H(\mathbf{v}_A \odot \mathbf{v}_B) &= \mathbf{S}_H(\mathbf{v}_A) \odot \mathbf{S}_H(\mathbf{v}_B)
\end{align*}
\]

Here, as elsewhere in this paper, \( \odot \) is Hadamard product.

In general, although it is mathematically convenient to define the behavior of sketches in reference to \( k \)-hot vectors, it is not necessary to construct a vector \( \mathbf{v}_A \) to construct a sketch: all that is needed is the non-zero weights of the elements of \( A \). Alternatively, if one precomputes and stores the sketch for each singleton set, it is possible to create sketches for an arbitrary set by gathering and sum-pooling the sketches for each element.

B.3 Probabilistic bounds on accuracy

We assume the hash functions are random mappings from \( \{1, \ldots, N\} \) to \( \{1, \ldots, N_W\} \). More precisely, we assume that for all \( i \in \{1, \ldots, N\} \), and all \( j \in \{1, \ldots, N_W\} \), \( \Pr(h_i(x) = a) = \frac{1}{N_W} \).

We will also assume that the \( N_D \) hash functions are are drawn independently at random. More precisely, for all \( i \neq i', i, i' \in \{1, \ldots, N\} \), all \( j, j' \in \{1, \ldots, N_D\} \) and all \( k, k' \in \{1, \ldots, N_W\} \), \( \Pr(h_j(i) = k \land h_j'(i') = k') = \frac{1}{N_W^2} \).

Under this assumption, the probability of errors can be easily bounded. Suppose the sketch width is at least twice the cardinality of \( A \), i.e., \( |A| < m \) and \( N_W > 2m \). Then one can show for all primitive sketches \( j \):

\[
\Pr(\mathbf{S}[j, h_j(i)] \neq \mathbf{v}_A[i]) \leq \frac{1}{2}
\]
leads to this result.

If $N^2 > \frac{2}{\epsilon}$ and $N_D > \log \frac{1}{\epsilon}$, the probability that $\text{CM}(i, S) > \text{v}_A[i] + \epsilon$ is no more than $\delta$ (Cormode and Muthukrishnan, 2005). Because there are many reasonable formal bounds that might or might not apply in an experimental setting, typically the sketch shape is treated as a hyperparameter to be optimized in experimental settings.

### C Implementation Details

#### C.1 Set difference

Another operation we use is set difference: e.g. “movie directors but not writers” requires one to compute a set difference $A_{\text{directors}} - B_{\text{writers}}$. In computing a set difference, the soft-type of the output $A - B$ is the same as that of $A$, and we exclude the necessary elements from the count-min sketch to produce $(a_{A - B}, b_{A - B})$, where

$$a_{A - B} = a_A$$
$$b_{A - B} = b_A \odot (b \neq 0)$$

This is exact when $B$ is unweighted (the case we consider here), but only approximates set difference for general weighted sets.
C.2 MetaQA

MetaQA makes use of the set difference operation. For example, to answer the question “What are other movies that have the same director as *Inception*?” we need to first find the director of *Inception*, Christopher Nolan, and all movies directed by him. Since the question above asks about other movies, the model should also remove the movie *Inception* from this set to obtain the final answer set $Y$. Thus in the first line of our model, we write

$$\hat{Y} = X_q \cdot \text{follow}(R_1) \cdot \text{follow}(R_2) - X_q$$

For MetaQA, the entity embedding is just a learned lookup table. The question representation $\text{encode}(q)$ is computed with a bag-of-word approach, i.e., an average pooling on the word embeddings of question $q$. The embedding size is 64, and scaling parameter for relation $\lambda$ is 1.0. Our count-min sketch has depth $N_D = 20$ and width $N_W = 500$. We set $k = 100$ to be the number of entities we retrieve at each step, and we pre-train KB embeddings as in §5.1 and fix the embeddings when training our QA model.

C.3 WebQuestionsSP

We use pre-trained BERT to encode our question $q$, i.e., $\text{encode}(q)$ is the BERT embedding of the [CLS] token. The relation sets $R_1$, $R_2$, $R_3$ are linear projections of the question embedding $\text{encode}(q)$ paired with a vacuous all-ones sketch $b_I$. Relation centroids are stacked with one extra dimension that encodes the hard-type of entities: here the hard-type is a binary value that indicates if the entity is a *cvt* node or not.

For this dataset, to make the relations entities easier to predict, the embedding of each entity is a learned transformation of the BERT encoding of the surface form of the entity names. In the experiments the BERT embeddings are transformed to 128 dimensions and the entity-specific portion $e^I_x$ has a dimension of 32. The scaling parameter for relation $\lambda$ is 0.1. The KB embedding is fixed after pre-training, using a procedure analogous to that of §5.1. We use a count-min sketch with depth $N_D = 20$ and width $N_W = 2000$, and we retrieve $k = 1000$ intermediate results at each step.

D More Results

D.1 Learn to reason with a KB

We run a quick experiment to test the reasoning ability of a popular pre-trained KB embedding, TransE (Bordes et al., 2013). We download the 64-dimension TransE embedding on FreeBase trained by Han et al. (2018)\(^{14}\) and evaluate the set representation task on the subset of FreeBase constructed for the WebQuestionsSP. The numbers are shown in Table 9, which shows that TransE embedding is not good for our retrieval purpose.

D.2 WebQuestionsSP

We did two more experiments on the WebQuestionsSP dataset. First, we remove the BERT pretrained embedding discussed in §3.3. Instead, we randomly initialize KB entity and relation embeddings, and train the set operations. The performance of EmQL (no-bert) on the downstream QA task is 1.3% lower than our full model. Second, we replace the exact MIPS with a fast maximal inner-product search (Mussmann and Ermon, 2016). This fast MIPS is an approximation of MIPS that eventually causes 2.1% drop in performance (Table 10).

\(^{14}\)Data available for download at https://github.com/thunlp/OpenKE.

|          | $k=1$ | $k=10$ | $k=100$ | $k=1000$ |
|----------|-------|--------|---------|----------|
| EmQL     | 18.4  | 72.6   | 94.3    | 97.8     |
| TransE   | 2.3   | 6.2    | 11.0    | 14.9     |

Table 9: Recall@k for set representation using 64-dimension EmQL and TransE embeddings on a subset of FreeBase

|          | WebQuestionsSP |
|----------|---------------|
| EmQL     | 75.5          |
| EmQL (no-sketch) | 53.2     |
| EmQL (no-constr)  | 65.2     |
| EmQL (approx. MIPS) | 73.4     |
| EmQL (no-bert)    | 74.2     |

Table 10: Ablated study on WebQuestionsSP