DIFFERENTIABLE REASONING OVER A VIRTUAL KNOWLEDGE BASE

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ABSTRACT

We consider the task of answering complex multi-hop questions using a corpus as a *virtual knowledge base (KB)*. In particular, we describe a neural module, DrKIT, that traverses textual data like a virtual KB, softly following paths of relations between *mentions* of entities in the corpus. At each step the operation uses a combination of sparse-matrix TFIDF indices and maximum inner product search (MIPS) on a special index of contextual representations. This module is differentiable, so the full system can be trained completely end-to-end using gradient based methods, starting from natural language inputs. We also describe a pretraining scheme for the index mention encoder by generating hard negative examples using existing knowledge bases. We show that DrKIT improves accuracy by 9 points on 3-hop questions in the MetaQA dataset, cutting the gap between text-based and KB-based state-of-the-art by 70%. DrKIT is also very efficient, processing upto 10x more queries per second than existing state-of-the-art QA systems.

1 INTRODUCTION

Large knowledge bases (KBs), such as FreeBase and Wikidata, organize information around *entities*, which makes it easy to reason over their contents. For example, given a query like *"When was Grateful Dead's lead singer born?"*, one can identify the entity `Grateful Dead` and the path of relations `LeadSinger, BirthDate` to efficiently extract the answer—provided that this information is present in the KB. Unfortunately, large KBs are often incomplete (Min et al., 2013). While relation extraction methods can be used to populate KBs, this process is inherently error-prone, and errors in extraction can propagate to downstream tasks.

Advances in open-domain QA (Moldovan et al., 2002; Yang et al., 2019) suggest an alternative—instead of performing relation extraction, one could *treat a large corpus as a virtual KB* by answering queries with spans from the corpus. This ensures facts are not lost in the relation extraction process, but also poses challenges. One challenge is that it is relatively expensive to answer questions using QA models which encode each document in a query-dependent fashion (Chen et al., 2017; Devlin et al., 2019)—even with modern hardware (Strubell et al., 2019; Schwartz et al., 2019). The cost of QA is especially problematic for certain complex questions, such as the example question above. If the passages stating that *"Jerry Garcia was the lead singer of Grateful Dead"* and *"Jerry Garcia was born in 1942"* are far apart in the corpus, it is difficult for systems that retrieve and read a single passage to find an answer—even though in this example, it might be easy to answer the question after the relations were explicitly extracted into a KB. More generally, *complex questions* involving sets of entities or paths of relations may require aggregating information from entity mentions in multiple documents, which is expensive.

One step towards efficient QA is the recent work of Seo et al. (2018; 2019) on *phrase-indexed question answering* (PIQA), in which spans in the text corpus are associated with question-independent contextual representations and then indexed for fast retrieval. Natural language questions are then answered by converting them into vectors that are used to perform inner product search (MIPS) against the index. This ensures efficiency during inference. However, this approach cannot be directly used to answer *complex* queries, since by construction, the information stored in the index is about the *local* context around a span—it can only be used for questions where the answer can be derived by reading a *single* passage.

This paper addresses this limitation of phrase-indexed question answering. We introduce an efficient, end-to-end differentiable framework for doing complex QA over a large text corpus that has been

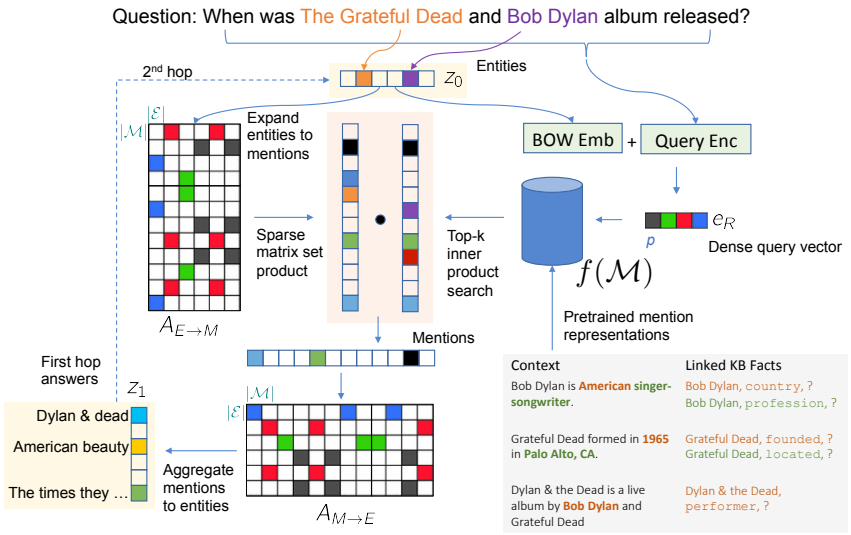

Figure 1: DrKIT answers multi-hop questions by iteratively mapping an input set of entities X (`The Grateful Dead`,`Bob Dylan`) to an output set of entities Y (`Dylan & Dead`, `American beauty`, ...) which are related to any input entity by some relation R (`album by`).

encoded in a query-independent manner. Specifically, we consider "multi-hop" complex queries which can be answered by repeatedly executing a "soft" version of the operation below, defined over a set of entities X and a relation R:

$$Y = X.\text{follow}(R) = \{x' : \exists x \in X \text{ s.t. } R(x, x') \text{ holds}\}$$

In past work soft, differentiable versions of this operation were used to answer multi-hop questions against an explicit KB (Cohen et al., 2019). Here we propose a more powerful neural module which approximates this operation against an indexed corpus In our module, the input X is a sparse vector representing a weighted set of entities, and the relation R is a dense feature vector, e.g. a vector derived from a neural network over a natural language query. The output Y is another sparse vector representing the weighted set of entities, aggregated over entity mentions in the top-k spans retrieved from the index. The spans in turn are retrieved using a MIPS query constructed from X and R, and we discuss pretraining schemes for the index in §2.3.

For multi-hop queries, the output entities Y can be recursively passed as input to the next iteration of the same module. The weights of the entities in Y are differentiable w.r.t the MIPS queries, which allows end-to-end learning *without* any intermediate supervision. We discuss an implementation based on sparse matrix-vector products, whose runtime and memory depend *only* on the number of spans K retrieved from the index. This is crucial for scaling up to large corpora, and leads to upto 15x faster inference than existing state-of-the-art multi-hop and open-domain QA systems. The system we introduce is called DrKIT (for Differentiable Reasoning over a Knowledge base of Indexed Text). We test DrKIT on the MetaQA benchmark for complex question answering, and show that it improves on prior text-based systems by 5 points on 2-hop and 9 points on 3-hop questions, reducing the gap between text-based ad KB-based systems by 30% and 70%, respectively. We also test DrKIT on a new dataset of multi-hop slot-filling over Wikipedia articles, and show that it outperforms DrQA (Chen et al., 2017) and PIQA (Seo et al., 2019) adapted to this task.

2 Differentiable Reasoning over a KB of Indexed Text

We want to answer a question q using a text corpus as if it were a KB. We start with the set of entities z in the question q and would ideally want to follow relevant outgoing relation edges in the KB to arrive at the answer. To simulate this behaviour on text, we first expand z to set of co-occurring mentions (say using TF-IDF) m. Not all of these co-occurring mentions are relevant for the question q, so we train a neural network which filters the mentions based on a relevance score of q to m. Then we can aggregate the resulting set of mentions m to the entities they refer to end up with an ordered set z' of entities which are answer candidates, very similar to traversing the KB. Furthermore, if the question requires more than one hop to answer, we can repeat the above procedure starting with z'. This is depicted pictorially in Figure 1.

We begin by first formalizing this idea in §2.1 in a probabilistic framework. In §2.2, we describe how the expansion of entities to mentions and the filtering of mentions can be performed efficiently, using sparse matrix products, and MIPS algorithms (Johnson et al., 2017). Lastly we discuss a pretraining scheme for constructing the mention representations in §2.3.

Notation: We denote the given corpus as $\mathcal{D} = \{d_1, d_2, \ldots\}$, where each $d_k = (d_k^1, \ldots, d_k^{L_k})$ is a sequence of tokens. We start by running an entity linker over the corpus to identify mentions of a fixed set of entities $\mathcal{E}$. Each mention m is a tuple (e_m, k_m, i_m, j_m) denoting that the text span $d_{k_m}^{i_m}, \ldots, d_{k_m}^{j_m}$ in document k_m mentions the entity $e_m \in \mathcal{E}$, and the collection of all mentions in the corpus is denoted as $\mathcal{M}$. Note that typically $|\mathcal{M}| \gg |\mathcal{E}|$.

2.1 Differentiable Multi-Hop Reasoning

We assume a *weakly supervised* setting where during training we only know the final answer entities $a \in \mathcal{E}$ for a T-hop question. We denote the latent sequence of entities which answer each of the intermediate hops as $z_0, z_1, \ldots, z_T \in \mathcal{E}$, where z_0 is mentioned in the question, and $z_t = a$. We can recursively write the probability of an intermediate answer as:

$$\Pr(z_t|q) = \sum_{z_{t-1} \in \mathcal{E}} \Pr(z_t|q, z_{t-1}) \Pr(z_{t-1}|q) \tag{1}$$

Here $\Pr(z_0|q)$ is the output of an entity linking system over the question, and $\Pr(z_t|q, z_{t-1})$ corresponds to a single-hop model which answers the t-th hop, *given* the entity from the previous hop z_{t-1}, by following the appropriate relation. Eq. 1 models reasoning over a chain of latent entities, but when answering questions over a text corpus, we must reason over entity *mentions*, rather than entities themselves. Hence $\Pr(z_t|q, z_{t-1})$ needs to be aggregated over all mentions of z_t, which yields

$$\Pr(z_t|q) = \sum_{m \in \mathcal{M}} \sum_{z_{t-1} \in \mathcal{E}} \Pr(z_t|m) \Pr(m|q, z_{t-1}) \Pr(z_{t-1}|q) \tag{2}$$

The interesting term to model in the above equation is $Pr(m|q, z_{t-1})$, which represents the relevance of mention m given the question about entity z_{t-1}. Following the analogy of a KB, we first expand the entity z_{t-1} to co-occuring mentions m and use a learnt scoring function to find the relevance of these mentions. Formally, let $F(m)$ denote a TF-IDF vector for the document containing m, $G(z_{t-1})$ be the TF-IDF vector of the *surface form* of the entity from the previous hop, and $s(m, q, z)$ be a learnt scoring function. Thus, we model $\Pr(m|q, z_{t-1})$ as

$$\Pr(m|q, z_{t-1}) \propto \underbrace{\mathbb{1}\{G(z_{t-1}) \cdot F(m) > \epsilon\}}_{\text{expansion to co-occurring mentions}} \times \underbrace{s(m, z_{t-1}, q)}_{\text{relevance filtering}} \tag{3}$$

Another equivalent way to look at our model in Eq. 3 is that the second term retrieves mentions of the correct *type* requested by the question in the t-th hop, and the first term filters these based on co-occurrence with z_{t-1}. When dealing with a large set of mentions m, we will typically retain only the top-k relevant mentions. We will show that this joint modelling of co-occurrence and relevance is important for good performance, which has also been observed in past (Seo et al., 2019).

The other term left in Eq. 2 is $\Pr(z|m)$, which is 1 if mention m matches the entity z else 0, since each mention can only point to a single entity. In general, to compute Eq. 2 the mention scoring of Eq. 3 needs to be evaluated for all latent entity and mention pairs, which is prohibitively expensive. However, by restricting s to be an inner product we can implement this efficiently (§2.2).

To highlight the differentiability of the proposed overall scheme, we can represent the computation in Eq. 2 as matrix operations. We pre-compute the TFIDF term for all entities and mentions into a *sparse* matrix, which we denote as $A_{E \to M}[e, m] = \mathbb{1}\left(G(e) \cdot F(m) > \epsilon\right)$. Then entity expansion to co-occuring mentions can be considered to be a sparse-matrix by sparse-vector multiplication between $A_{E \to M}$ and z_{t-1}. For the relevance scores, let $\mathbb{T}_K(s(m, z_{t-1}, q))$ denote the top-K relevant mentions encoded as a *sparse* vector in $\mathbb{R}^{|\mathcal{M}|}$. Finally, the aggregation of mentions to entities can be formulated as multiplication with another sparse matrix $A_{M \to E}$, which encodes *coreference*, i.e. mentions corresponding to the same entity. Putting all these together, using $\odot$ to denote element-wise product, and defining $Z_t = [\Pr(z_t = e_1|q); \ldots; \Pr(z_t = e_{|\mathcal{E}|}|q)]$, we can observe that for large K (i.e., as $K \to |\mathcal{M}|$), eq. (2) becomes equivalent to:

$$Z_t = \text{softmax}\left(\left[Z_{t-1}^T A_{E \to M} \odot \mathbb{T}_K(s(q, m, z_{t-1}))\right] A_{M \to E}\right). \tag{4}$$

Note that *every operation in above equation is differentiable and between sparse matrices and vectors*: we will discuss efficient implementations in §2.2. Further, the number of non-zero entries in Z_t is bounded by K, since we filtered (the multiplication in Eq. 4) to top-k relevant mentions among TF-IDF based expansion and since each mention can only point to a single entity in $A_{M \to E}$. This is important, as it prevents the number of entries in Z_t from exploding across hops (which might happen if, for instance, we added the dense and TF-IDF retrievals instead).

We can view Z_{t-1}, Z_t as weighted multisets of entities, and $g_t(q)$ as implicitly representing a relation R. Then Eq. 4 becomes a differentiable implementation of $Z_t = Z_{t-1}.\text{follow}(R)$, i.e. mimicking the graph traversal in a traditional KB. We thus call Eq. 4 a *textual follow operation*.

Training and Inference. The model is trained completely end-to-end by optimizing the cross-entropy loss between Z_T, the weighted set of entities after T hops, and the ground truth answer set A. We use a temperature coefficient λ when computing the softmax in Eq, 4. Finally, we also found that taking a *maximum* over the mention set of an entity M_{z_t} in Eq. 2 works better in practice than taking a sum. This corresponds to optimizing only over the most confident mention of each entity, which works for corpora like Wikipedia which do not have much redundancy of information. A similar observation has been made by Min et al. (2019) in weakly supervised settings.

2.2 Efficient Implementation

Sparse TF-IDF Mention Encoding. To compute the sparse $A_{E \to M}$ for entity-mention expansion in Eq. 4, the TF-IDF vectors $F(m)$ and $G(z_{t-1})$ are constructed over unigrams and bigrams, hashed to a vocabulary of $16M$ buckets. While F computes the vector from the whole passage around m, G only uses the surface form of z_{t-1}. This corresponds to retrieving all mentions in a document retrieved using z_{t-1} as the query. We limit the number of retrieved mentions per entity to a maximum of μ, which leads to a $|\mathcal{E}| \times |\mathcal{M}|$ sparse matrix.

Efficient Entity-Mention expansion. The expansion from a set of entities to mentions occurring around them can be computed using the sparse-matrix by sparse vector product $Z_{t-1}^T A_{E \to M}$. A simple lower bound for multiplying a sparse $|\mathcal{E}| \times |\mathcal{M}|$ matrix, with maximum μ non-zeros in each row, by a sparse $|\mathcal{E}| \times 1$ vector with k nonzeros is $\Omega(k\mu)$. Note that this lower bound is independent of the size of matrix $A_{E \to M}$ or in other words independent of number of entities or mentions. To attain the lower bound, the multiplication algorithm must be vector driven, because any matrix-driven algorithms need to at least iterate over all the rows. Instead we *slice* out the relevant rows from $A_{E \to M}$. To enable this our solution is to represent the sparse matrix $A_{E \to M}$ as two row-wise lists of a variable-sized lists of the non-zero elements index and values. This results in a ragged representation of the matrix which can be easily sliced corresponding to the non-zero entries in the vector in $O(\log E)$ time. We are now left with k sparse vectors with at most μ non-zero elements in each. We can add these k sparse vectors weighted by corresponding values from vector z in $O(k \max\{k, \mu\})$ time. Moreover, such an implementation is feasible with deep learning frameworks such as Tensorflow[1]. We quickly test the scalability of our approach by varying the number of entities for a fixed density of mentions μ (from Wikipedia). Figure 2 compared our approach to the default sparse-matrix times dense vector product (no sparse matrix times sparse vector is available in TensorFlow)[2].

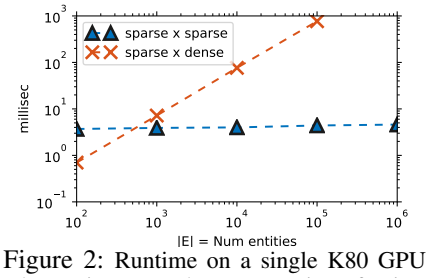

Figure 2: Runtime on a single K80 GPU when using ragged representations for implementing sparse matrix vector product, vs the default sparse matrix times dense vector product available in TensorFlow. $|\mathcal{E}| > 10^5$ leads to OOM for the latter.

Efficient top-k mention relevance filtering: To make computation of Eq. 4 feasible, we need an efficient way to get top-k relevant mentions of entity z_{t-1} for given question q, without enumerating all possibilities. A key insight is that by restricting scoring function $s(m, z_{t-1}, q)$ to an inner product, we can easily approximate a parallel version of this computation, across all mentions m. To do this, let $f(m)$ be a dense encoding of m, and $g_t(q, z_{t-1})$ be a dense encoding of the question q for the t-th hop, both in $\mathbb{R}^p$ (the details of the dense encoding is provided in next paragraph), then the scoring

[1] https://www.tensorflow.org/guide/ragged_tensors

[2] We will release our code publicly on acceptance.

function $s(m, z_{t-1}, q)$ becomes

$$s(m, z_{t-1}, q) \propto \exp\left\{f(m) \cdot g_t(q, z_{t-1})\right\}, \tag{5}$$

which can be computed in parallel by multiplying a matrix $f(\mathcal{M}) = [f(m_1); f(m_2); \ldots]$ with $g_t(q, z_{t-1})$. Although this matrix will be very large for a realistic corpus, but since eventually we are only interested in top-k values we can use an approximate algorithm for Maximum Inner Product Search (MIPS) (Andoni et al., 2015; Shrivastava & Li, 2014) to find the k top-scoring elements. The complexity of this filtering step using MIPS is roughly $O(kp \operatorname{polylog}|\mathcal{M}|)$.

Mention and Question Encoders. Mentions are encoded by passing the passages they are contained in through a BERT-large (Devlin et al., 2019) model (trained as described in § 2.3). Suppose mention m appears in passage d, starting at position i and ending at position j. Then $f(m) = W^T[H^d_i; H^d_j]$, where H^d is the sequence of embeddings output from BERT, and W is a linear projection to size p. The query are encoded with a smaller BERT-like model: specifically, it is tokenized with WordPieces (Schuster & Nakajima, 2012), appended to a special `[CLS]` token, and then passed through a 4-layer Transformer network (Vaswani et al., 2017) with the same architecture as BERT, producing an output sequence H^q. The g_t functions are defined similarly to the BERT model used for SQuAD-style QA. For each hop $t = 1, \ldots, T$, we add two addition Transformer layers on top of H^q, which will be trained to produce MIPS queries from the `[CLS]` encoding; the first added layer produces a MIPS query H^q_{st} to retrieve a start token, and the second added layer a MIPS query H^q_{en} to retrieve an end token. We concatenate the two and define $\tilde{g}_t(q) = V^T[H^q_{st}; H^q_{en}]$. Finally, to condition on current progress we add the embeddings of z_{t-1}. Specifically, we use entity embeddings $E \in \mathbb{R}^{|\mathcal{E}| \times p}$, to construct an average embedding of the set Z_{t-1}, as $Z^T_{t-1}E$, define $g_t(q, z_{t-1}) \equiv \tilde{g}_t(q) + Z^T_{t-1}$. To avoid a large number of parameters in the model, we compute the entity embeddings as an average over the word embeddings of the tokens in the entity's surface form. The computational cost of the question encoder $g_t(q)$ is $O(p^2)$.

Thus our total computational complexity to answer a query is $\tilde{O}(k \max\{k, \mu\} + kp + p^2)$ (almost independent to number of entities or mentions!), with $O(\mu|\mathcal{E}| + p|\mathcal{M}|)$ memory to store the precomputed matrices and mention index.[3]

2.3 Pretraining the Index

Ideally, we would like to train the mention encoder $f(m)$ end-to-end using labeled QA data only. However, this poses a challenge when combined with approximate nearest neighbor search—since after every update to the parameters of f, one would need to recompute the embeddings of all mentions in $\mathcal{M}$. We thus adopt a staged training approach: we first pre-train a mention encoder $f(m)$, then compute compute and index embeddings for all mentions once, keeping these embeddings fixed when training the downstream QA task. Empirically, we observed that using BERT representations "out of the box" do not capture the kind of information our task requires (Appendix §C), and thus, pretraining the encoder to capture better mention understanding is a crucial step.

One option adopted by previous researchers (Seo et al., 2018) is to fine-tune BERT on Squad (Rajpurkar et al., 2016). However, Squad is limited to only 536 articles from Wikipedia, leading to a very specific distribution of questions, and is not focused on entity- and relation-centric questions. Here we instead train the mention encoder using distant supervision from the KB.

Specifically, assume we are given an open-domain KB consisting of facts (e_1, R, e_2) specifying that the relation R holds between the subject e_1 and the object e_2. Then for a corpus of entity-linked text passages $\{d_k\}$, we automatically identify tuples $(d, (e_1, R, e_2))$ such that d mentions both e_1 and e_2. Using this data, we learn to answer slot-filling queries in a reading comprehension setup, where the query q is constructed from the surface form of the subject entity e_1 and a natural language description of R (e.g. "Jerry Garcia, birth place, ?"), and the answer e_2 needs to be extracted from the passage d. Using string representations in q ensures our pre-training setup is similar to the downstream task. In pretraining, we use the same scoring function as in previous section, but over all *spans* m in the passage:

$$s(m, e_1, q) \propto \exp\left\{f(s) \cdot g(q, e_1)\right\}. \tag{6}$$

Following Seo et al. (2016), we normalize start and end probabilities of the span separately.

[3]Following standard convention, in $\tilde{O}$ notation we suppress poly log dependence terms.

MetaQA			
Model	**1hop**	**2hop**	**3hop**
DrQA (ots)	0.553	0.325	0.197
KVMem†	0.762	0.070	0.195
GraftNet†	0.825	0.362	0.402
PullNet†	0.844	0.810	0.782
DrKIT (e2e)	0.844	0.860	**0.876**
DrKIT (strong sup.)	**0.845**	**0.871**	0.871

WikiData			
Model	**1hop**	**2hop**	**3hop**
DrQA (ots, cascade)	0.287	0.141	0.070
PIQA (ots, cascade)	0.240	0.118	0.064
PIQA (pre, cascade)	0.670	0.369	0.182
DrKIT (pre, cascade)	0.816	0.404	0.198
DrKIT (e2e)	**0.834**	**0.469**	**0.244**
–BERT index	0.643	0.294	0.165

Table 1: **(Left)** MetaQA and **(Right)** WikiData Hits @1 for 1-3 hop sub-tasks. ots: off-the-shelf without re-training. †: obtained from Sun et al. (2019). cascade: adapted to multi-hop setting by repeatedly applying Eq. 2. pre: pre-trained on slot-filling. e2e: end-to-end trained on single-hop and multi-hop queries.

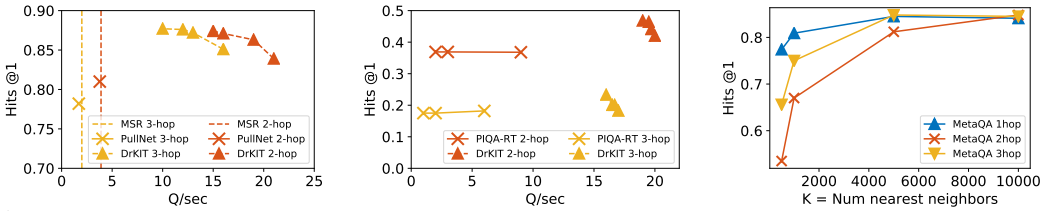

Figure 3: Hits @1 vs Queries/sec during inference on **(Left)** MetaQA and **(Middle)** WikiData tasks, measured on a single CPU server with 6 cores. **(Right)** Effect of varying number of nearest neighbors K during MIPS.

For effective transfer to the full corpus setting, we must also provide negative instances during pre-training, i.e. query and passage pairs where the answer is *not contained* in the passage. We consider three types of hard negatives: (1) *Shared-entity negatives*, which pair a query $(e_1, R, ?)$ with a passage which mentions e_1 but not the correct tail answer. (2) *Shared-relation negative*, which pair a query $(e_1, R, ?)$ with a passage mentioning two other entities e'_1 and e'_2 in the same relation R. (3) *Random negatives*, which pair queries with random passages from the corpus.

For the multi-hop slot-filling, we used Wikidata (Vrandečić & Krötzsch, 2014) as our KB, Wikipedia as the corpus, and SLING (Ringgaard et al., 2017) to identify entity mentions. We add the restriction that d must be from the Wikipedia article of the subject entity to reduce noise. Overall we collected $950K$ pairs over $550K$ articles. For the experiments with MetaQA, we supplemented this data with the corpus and KB provided with MetaQA, and string matching for entity linking.

3 Experiments

3.1 MetaQA: Multi-Hop Question Answering with Text

Dataset. We first evaluate DrKIT on the MetaQA benchmark for multi-hop question answering (Zhang et al., 2018). METAQA consists of around $400K$ questions ranging from 1 to 3 hops constructed by sampling relation paths from a movies KB (Miller et al., 2016) and converting them to natural language using templates. The questions cover 8 relations and their inverses, around $43K$ entities, and are paired with a corpus consisting of $18K$ Wikipedia passages about those entities. The questions are all designed to be answerable using either the KB or the corpus, which makes it possible to compare the performance of our "virtual KB" QA system to a plausible upper bound system that has access to a complete KB. We used the same version of the data as Sun et al. (2019). Details of implementation MetaQA is in Appendix A

Results. Table 1 shows the accuracy of the top-most retrieved entity (Hits@1) for the sub-tasks ranging from 1-3 hops, and compares to the state-of-the-art systems for the text-only setting on these tasks. DrKIT outperforms the prior state-of-the-art by a large margin in the 2-hop and 3-hop cases. The strongest prior method, PullNet (Sun et al., 2019; 2018), uses a graph neural network model with learned iterative retrieval from the corpus to answer multi-hop questions. It uses the MetaQA KB during training to identify shortest paths between the question entity and answer entity, which are used to supervise the text retrieval and reading modules. DrKIT, on the other hand, has strong performance without such supervision, demonstrating its capability for end-to-end learning. (Adding

the same intermediate supervision to DrKIT does not even consistently improve performance—it gives DrKIT a small lift on 1- and 2-hop questions but does not help for 3-hop questions.)

DrKIT's architecture is driven, in part, by efficiency considerations: unlike PullNet, it is designed to answer questions with minimal processing at query time. Figure 3 compares the tradeoffs between accuracy and inference time of DrKIT with PullNet as we vary K, the number of dense nearest neighbors retrieved. The runtime gains of DrKIT over PullNet range between 5x-15x.

Analysis. We perform ablations on DrKIT for the MetaQA data. First, we empirically confirm that taking a sum instead of max over the mentions of an entity hurts performance. So does removing the softmax temperature (by setting $\lambda = 1$). Removing the TFIDF component from Eq. 3, leads a large decrease in performance for 2-hop and 3-hop questions. This is because the TFIDF component *constrains* the end-to-end learning to be along reasonable paths of co-occurring mentions; otherwise the search space becomes too large. The results also highlight the importance of pretraining method introduced in §2.3, as DrKIT over an index of BERT representations without pretraining is 23 points worse in the 3-hop case. We also check the performance when the KB used for pre-training is *incomplete*. Even with only 25% edges retained, we see a high performance, better than PullNet, and far better than state-of-the-art KB-only methods.

Ablations	**1hop**	**2hop**	**3hop**
DrKIT	0.844	0.86	0.876
–Sum over M_{z_t}	0.837	0.823	0.797
$-\lambda = 1$	0.836	0.752	0.799
–w/o TFIDF	0.845	0.548	0.488
–BERT index	0.634	0.610	0.555
Incomplete KB for pretraining			
25% KB	0.839	0.804	0.830
50% KB	0.843	0.834	0.834
(50% KB-only)	*0.680*	*0.521*	*0.597*

3.2 WIKIDATA: MULTI-HOP SLOT-FILLING

The MetaQA dataset has been fairly well-studied, but has limitations since it is constructed over a small KB. In this section we consider a new task, in a larger scale setting with many more relations, entities and text passages. The new dataset also lets us evaluate performance in a setting where the test set contains documents and entities not seen at training time, an important issue when devising a QA system that will be used in a real-world setting, where the corpus and entities in the discourse change over time, and lets us perform analyses not possible with MetaQA, such as extrapolating from single-hop to multi-hop settings without retraining.

Dataset. We sample two subsets of Wikipedia articles, one for pre-training (§2.3) and end-to-end training, and one for testing. For each subset we consider the set of WikiData entities mentioned in the articles, and sample paths of 1-3 hop relations among them, ensuring that any intermediate entity has an in-degree of no more than 100. Then we construct a semi-structured query by concatenating the surface forms of the head entity with the path of relations (e.g. "Helene Gayle, employer, founded by, ?"). The answer is the tail entity at the end of the path, and the task is to extract it from the Wikipedia articles. Existing slot-filling tasks (Levy et al., 2017; Surdeanu, 2013) focus on a *single-hop*, *static* corpus setting, whereas our task considers a *dynamic* setting which requires to travers the corpus. For each setting, we create a dataset with $10K$ articles, $120K$ passages, $> 200K$ entities and $1.5M$ mentions, resulting in an index of size about 2gb. We include example queries in Appendix.

Baselines. We adapt two publicly available open-domain QA systems for this task – DrQA[4] (Chen et al., 2017) and PIQA[5] (Seo et al., 2019). While DrQA is relatively mature and widely used, PIQA is recent, and similar to our setup since it also answers questions with minimal computation at query time. It is broadly similar to a single textual follow operation in DrKIT, but is not constructed to allow retrieved answers to be converted to entities and then used in subsequent processing, so it is not directly applicable to multi-hop queries. We thus also consider a cascaded architecture which repeatedly applies Eq. 2, using either of PIQA or DrQA to compute $\Pr(z_t|q, z_{t-1})$ against the corpus, retaining at most k intermediate answers in each step. We tune k in the range of 1-10, since larger values make the runtime infeasible. Further, since these models were trained on natural language questions, we use the templates released by Levy et al. (2017) to convert intermediate questions into natural text.[6] We test off-the-shelf versions of these systems, as well as a version of PIQA re-trained

[4] `https://github.com/facebookresearch/DrQA`

[5] `https://github.com/uwnlp/denspi`

[6] For example, "Helene Gayle. employer?" becomes "Who is the employer of Helene Gayle?"

on our our slot-filling data.[7] We compare to a version of DrKIT trained only on single-hop queries (§2.3) and similarly cascaded, and one version trained end-to-end on the multi-hop queries.

Results. Table 1 (right) lists the Hits @1 performance on this task. Off-the-shelf open-domain QA systems perform poorly, showing the challenging nature of the task. Re-training PIQA on the slot-filling data improves performance considerably, but DrKIT trained on the same data improves on it. A large improvement is seen on top of these cascaded architectures by end-to-end training, which is made possible by the differentiable operation introduced in this paper. We also list performance of DrKIT when trained against an index of fixed BERT-large mention representations. While this is comparable to the re-trained version of PIQA, it lags behind DrKIT pre-trained using the KB, once again highlighting the importance of the scheme outlined in §2.3. We also plot the Hits @1 against Queries/sec for cascaded versions of PIQA and DrKIT in Figure 3 (middle). We observe gains of 2x-3x to DrKIT, due to the efficient implementation of entity-mention expansion discussed in §2.2.

Analysis. In order to understand where the accuracy gains for DrKIT come from, we conduct experiments on the dataset of slot-filling queries released by Levy et al. (2017). We construct an *open* version of the task by collecting Wikipedia articles of all subject entities in the data. A detailed discussion is in Appendix C, here we note the main findings. PIQA trained on Squad only gets 30% macro-avg accuracy on this data, but this improves to 46% when re-trained on our slot-filling data. Interestingly, a version of DrKIT which selects from *all spans* in the corpus performs similarly to PIQA (50%), but when using entity linking it significantly improves to 66%. It also has 55% accuracy in answering queries about *rare* relations, i.e. those observed < 5 times in its training data. We also conduct probing experiments comparing the representations learned using slot-filling to those by vanilla BERT. We found that while the two are comparable in detecting *fine-grained entity types*, the slot-filling version is significantly better at encoding *entity co-occurrence* information.

4 Related Work

Neural Query Language (NQL) (Cohen et al., 2019) defines differentiable templates for multi-step access to a symbolic KB, in which relations between entities are *explicitly* enumerated. Here, we focus on the case where the relations are implicit in mention representations derived from text. Knowledge Graph embeddings (Bordes et al., 2013; Yang et al., 2014; Dettmers et al., 2018) attach continuous representations to discrete symbols which allow them to be incorporated in deep networks (Yang & Mitchell, 2017). Embeddings often allow generalization to unseen facts using relation patterns, but text corpora are more complete in the information they contain.

Talmor & Berant (2018) also examined answering compositional questions by treating a text corpus (in their case the entire web) as a KB. However their approach consists of parsing the query into a computation tree separately, and running a black-box QA model on its leaves separately, which *cannot* be trained end-to-end. Recent papers have also looked at complex QA using graph neural networks (Sun et al., 2018; Cao et al., 2019; Xiao et al., 2019) or by identifying paths of entities in text (Jiang et al., 2019; Kundu et al., 2019; Dhingra et al., 2018). These approaches rely on identifying a small relevant pool of evidence documents containing the information required for multi-step QA. Hence, Sun et al. (2019) and Ding et al. (2019), incorporate a dynamic retrieval process to add text about entities identified as relevant in the previous layer of the model. Since the evidence text is processed in a query-dependent manner, the inference speed is slower than when it is pre-processed into an indexed representation (see Figure 3). The same limitation is shared by methods which perform multi-step retrieval interleaved with a reading comprehension model (Das et al., 2019; Feldman & El-Yaniv, 2019; Lee et al., 2019).

5 Conclusion

We present DrKIT, a differentiable module that is capable of answering multi-hop questions directly using a large entity-linked text corpus. DrKIT is designed to imitate traversal in KB over the text corpus, providing ability to follow relations in the "virtual" KB over text. We achieve state-of-the-art results on MetaQA dataset for answering natural language questions, with a 9 point increase in the 3-hop case. We also developed an efficient implementation using sparse operations and inner product search, which led to a 10x increase in QPS over baseline approaches.

[7] We tuned several hyperparameters of PIQA on our data, eventually picking the *sparse first* strategy, a sparse weight of 0.1, and a filter threshold of 0.2. For the Squad trained version, we also had to remove paragraphs smaller than 50 tokens since with these the model failed completely.

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A METAQA: IMPLEMENTATION DETAILS

We use $p = 400$ dimensional embeddings for the mentions and queries, and 200-dimensional embeddings each for the start and end positions. This results in an index of size 750MB. When computing $A_{E \to M}$, the entity to mention co-occurrence matrix, we only retain mentions in the top 50 paragraphs matched with an entity, to ensure sparsity. Further we initialize the first 4 layers of the question encoder with the Transformer network from pre-training. For the first hop, we assign Z_0 as a 1-hot vector for the least frequent entity detected in the question using an exact match. The number of nearest neighbors K and the softmax temperature λ were tuned on the dev set of each task, and we found $K = 10000$ and $\lambda = 4$ to work best. We pretrain the index on a combination of the MetaQA corpus, using the KB provided with MetaQA for distance data, and the Wikidata corpus.

B WIKIDATA DATASET STATISTICS

Task	**#train**	**#dev**	**#test**	$\lvert\mathcal{E}_{test}\rvert$	$\lvert\mathcal{M}_{test}\rvert$	$\lvert\mathcal{D}_{test}$	**Example**
1hop	16901	2467	10000	216K	1.2M	120K	Q. Mendix, industry? A. Enterprise Software
2hop	163607	398	9897	342K	1.9M	120K	Q. 2000 Hel van het Mergelland, winner, place of birth? A. Bert Grabsch → Lutherstadt Wittenberg
3hop	36061	453	9899	261K	1.8M	120K	Q. Magnificent!, record label, founded by, date of death? A. Prestige → Bob Weinstock → 14 Jan 2006

Table 2: Wikidata dataset

Details of the collected WikiData dataset are shown in Table 2.

C INDEX ANALYSIS

Single-hop questions and relation extraction. Levy et al. (2017) released a dataset of $1M$ slot-filling queries of the form $(e_1, R, ?)$ paired with Wikipedia sentences mentioning e_1, which was used for training systems that answered single-step slot-filling questions based on a small set of candidate passages. Here we consider an *open* version of the same task, where answers to the queries must be extracted from a corpus rather than provided candidates. We construct the corpus by collecting and entity-linking all paragraphs in the Wikipedia articles of all $8K$ subject entities in the dev and test sets, leading to a total of $109K$ passages. After constructing the TFIDF $A_{E \to M}$ and coreference $A_{M \to E}$ matrices for this corpus, we directly use our pre-trained index to answer the test set queries.

Probing Task	Negative Example	BERT	DrKIT
Shared Entity	Neil Herron played for West of Scotland.	0.850	0.876
Shared Relation	William Paston was a British politician.	0.715	0.846

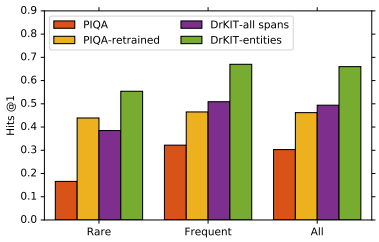

Figure 4: **Left:** Macro-avg accuracy on the Levy et al. (2017) relation extraction dataset. We split the results based on frequency of the relations in our WikiData training data. DrKIT-all spans refers to a variant of our model which selects from all spans in the corpus, instead of only entity-linked mentions. **Right:** F1 scores on Shared Entity and Shared Relation negatives. The negative context examples are for the Query : (Neil Herron, occupation, ?)

Figure 4 (Right) shows the Hits@1 performance of the Levy et al. (2017) slot-filling dataset. We report results on 2 subsets of relations in addition to all relations. The Rare subset comprises of relations with frequencies < 5 in the training data while the 'Frequent' subset contains the rest. DrKIT on entity-mentions consistently outperforms the other phrase-based models showing the benefit of indexing entity-mentions in single-hop questions over. Note that DrKit-entities has a high Hits@1 performance on the Rare relations subset, showing that there is generalization to less frequent data due to the natural language representations of entities and relations.

Probing Experiments Finally, to compare the representations learned by the BERT model fine-tuned on the Wikidata slot-filling task, we design two probing experiments. In each experiment, we keep the parameters of the BERT model (mention encoders) being probed fixed and only train the query encoders. Similar to Tenney et al. (2019), we use a weighted average of the layers of BERT here rather than only the top-most layer, where the weights are learned on the probing task.

In the first experiment, we train and test on shared-entity negatives. Good performance here means the BERT model being probed encodes fine-grained *entity-type* information reliably[8]. As shown in Table 4, BERT performs well on this task, suggesting it encodes fine-grained types well.

In the second experiment, we train and test only on shared-relation negatives. Good performance here means that the BERT model encodes *entity co-occurrence* information reliably. In this probe task, we see a large performance drop for Bert, suggesting it does not encode entity co-occurrence information well. The good performance of the DrKIT model on both experiments suggests that fine-tuning on the slot-filling task primarily helps the contextual representations to also encode entity co-occurrence information, in addition to entity type information.

[8]A reasonable heuristic for solving this task is to simply detect an entity with the correct type in the given sentence, since all sentences contain the subject entity.