Query Embedding on Hyper-relational Knowledge Graphs

Dimitrios Alivanistos  
Computer Science  
Vrije Universiteit Amsterdam  
Discovery Lab, Elsevier  
Amsterdam, the Netherlands  
d.alivanistos@vu.nl

Max Berrendorf  
Ludwig-Maximilians-Universität München  
Munich, Germany  
berrendorf@dbs.ifi.lmu.de

Michael Cochez  
Computer Science  
Vrije Universiteit Amsterdam  
Discovery Lab, Elsevier  
Amsterdam, the Netherlands  
m.cochez@vu.nl

Mikhail Galkin  
Mila & McGill University  
Montreal, Canada  
mikhail.galkin@mila.quebec

Abstract

Multi-hop logical reasoning is an established problem in the field of representation learning on knowledge graphs (KGs). It subsumes both one-hop link prediction as well as other more complex types of logical queries. Existing algorithms operate only on classical, triple-based graphs, whereas modern KGs often employ a hyper-relational modeling paradigm. In this paradigm, typed edges may have several key-value pairs known as qualifiers that provide fine-grained context for facts. In queries, this context modifies the meaning of relations, and usually reduces the answer set. Hyper-relational queries are often observed in real-world KG applications, and existing approaches for approximate query answering cannot make use of qualifier pairs. In this work, we bridge this gap and extend the multi-hop reasoning problem to hyper-relational KGs allowing to tackle this new type of complex queries. Building upon recent advancements in Graph Neural Networks and query embedding techniques, we study how to embed and answer hyper-relational conjunctive queries. Besides that, we propose a method to answer such queries and demonstrate in our experiments that qualifiers improve query answering on a diverse set of query patterns.

1 Introduction

Query embedding (QE) on knowledge graphs (KGs) aims to answer logical queries using neural reasoners instead of traditional databases and query languages. Traditionally, a KG is initially loaded into a database that understands a particular query language, e.g., SPARQL. The logic of a query is encoded into conjunctive graph patterns, variables, and common operators such as joins or unions.

On the other hand, QE bypasses the need for a database or query engine and performs reasoning directly in a latent space by computing a similarity score between the query representation and entity representation. A query representation is obtained by processing its equivalent logical formula

1Existing QE approaches operate only on the entity level and cannot have relations as variables.
where joins become intersections (\(\wedge\)), and variables are existentially quantified (\(\exists\)). A flurry of recent QE approaches \cite{13, 20, 19, 17, 2} expand the range of supported logical operators and graph patterns. However, all existing QE models work only on classical, triple-based KGs. In contrast, an increasing amount of publicly available \cite{29, 23} and industrial KGs adopt a hyper-relational modeling paradigm where typed edges may have additional attributes, in the form of key-value pairs, known as qualifiers. Several standardization efforts embody this paradigm, i.e., RDF* \cite{14} and Labeled Property Graphs (LPG)\cite{2}, with their query languages SPARQL* and GQL, respectively. Such hyper-relational queries involving qualifiers are instances of higher-order logical queries, and so far, there has been no attempt to bring neural reasoners to this domain.

In this work, we bridge this gap and propose a neural framework to extend the QE problem to hyper-relational KGs enabling answering more complex queries. Specifically, we focus on logical queries that use conjunctions (\(\wedge\)) and existential quantifiers (\(\exists\)), where the function symbols are parameterized with the qualifiers of the relation. This parameterization enables us (cf. Fig. 1) to answer queries like "What is the university \(U\) where the one who discovered the law of the photoelectric effect \(L\) got his/her BSc. degree?", which can be written as \(\exists U : \exists P.\ discovered\_by(L, P) \wedge educated\_at(\{\text{degree: BSc}\})(P, U)\).

Our contributions towards this problem are four-fold. First, as higher-order queries are intractable at practical scale, we show how to express such queries in terms of a subset of first-order logic (FOL) well-explored in the literature. Second, we build upon recent advancements in Graph Neural Networks (GNNs) and propose a method to answer conjunctive hyper-relational queries in a latent space. Then, we validate our approach by demonstrating empirically that qualifiers significantly improve query answering accuracy on a diverse set of query patterns. Finally, we show the robustness of our hyper-relational query answering model to two reification mechanisms commonly used in graph databases to store such graphs on a physical level.\(^\text{3}\)

2 Related Work

**Query Embedding.** The foundations of neural query answering and query embeddings laid in GQE \cite{13} considered conjunctive (\(\wedge\)) queries with existential (\(\exists\)) quantifiers modeled as geometric operators based on Deep Sets \cite{31}. Its further extension, QUERY2Box \cite{20}, proposed to represent queries as hyper-rectangles instead of points in a latent space. Geometrical operations on those rectangles allowed to answer queries with disjunction (\(\vee\)) re-written in the Disjunctive Normal Form (DNF). Changing the query representation form to beta distributions enabled BetaE \cite{19} to tackle

\(^\text{3}\)The source code for the model and our experiments can be found from https://github.com/DimitrisAlivas/StarQE.
queries with negation (¬). Another improvement over QUERY2BOX as to answering entailment queries was suggested in EMLQ [24] by using count-min sketches.

The other family of approaches represents queries as Directed Acyclic Graphs (DAGs). MPQE [8] assumes variables and targets as nodes in a query graph and applies an R-GCN [22] encoder over it. It was shown that message passing demonstrates promising generalization capabilities (i.e., when training only on 1-hop queries and evaluating on more complex patterns). Additional gains are brought when the number of R-GCN layers is equal to the graph diameter. Treating the query DAG as a fully-connected (clique) graph, BiQE [17] applied a Transformer encoder [27] and allowed to answer queries with multiple targets at different positions in a graph.

Finally, CQD [4] showed that it is possible to answer complex queries without an explicit query representation. Instead, CQD decomposes a query in a sequence of reasoning steps and performs a beam search in a latent space of KG embeddings models pre-trained on a simple 1-hop link prediction task. A particular novelty of this approach is that no end-to-end training on complex queries is required, and any trained embedding model of the existing abundance [16] can be employed as is.

Still, all of the described approaches are limited to triple-based KGs while we extend the QE problem to the domain of hyper-relational KGs. As our approach is also based on query graphs, we adopt and further study some of MPQE observations as to query diameter and generalization.

Hyper-relational KG Embedding. Due to its novelty, embedding hyper-relational KG is a field of ongoing research. Most of the few existing models are end-to-end decoder-only CNNs [21,22] limited to 1-hop link prediction, i.e., embeddings of entities and relations are stacked and passed through a CNN to score a statement. On the encoder side, we are only aware of STARE [11] to work in the hyper-relational setting. STARE extends the message passing framework of CompGCN [26] by composing qualifiers and aggregating their representations with the primary relation of a statement.

Inspired by the analysis of [21], we take a closer look at comparing hyper-relational queries against their reified counterparts (transformed into a triple-only form). We also adopt STARE [11] as a basic query graph encoder and further extend it with attentional aggregators akin to GAT [28].

3 Hyper-relational Knowledge Graphs and Queries

Definition 3.1 (Hyper-relational Knowledge Graph). Given a finite set of entities $E$, and a finite set of relations $R$, let $\Omega = 2^{(R \times E)}$. Then, we define a hyper-relational knowledge graph as $G = (E, R, S)$, where $S \subseteq (E \times R \times E \times \Omega)$ is a set of (qualified) statements.

For a single statement $s = (h, r, t, qp)$, we call $h, t \in E$ the head and tail entity, and $r \in R$ the (main) relation. This also indicates the direction of the relation from head to tail. The triple $(h, r, t)$ is also called the main triple. $qp = \{q_1, \ldots\} = \{(q_{r_1}, q_{e_1}), \ldots\} \subseteq R \times E$ is the set of qualifier pairs, where $\{q_{r_1}, q_{r_2}, \ldots\}$ are the qualifier relations and $\{q_{e_1}, q_{e_2}, \ldots\}$ the qualifier values.

Hyper-relational KGs extend traditional KGs by enabling to qualify triples. In this work, we solely use hyper-relational KGs and hence use KG to denote this variant. The qualifier pair set provides additional information for the semantic interpretation of the main triple $(h, r, t)$. For instance, consider the statement (AlbertEinstein, educated_at, ETHZurich, (degree, BSc))). Here, the qualifier pair (degree, BSc) gives additional context on the base triple (AlbertEinstein, educated_at, ETHZurich) (also illustrated on Fig. 1).

Note that this statement can equivalently be written in first order logic (FOL). Specifically, we can write it as a statement with a parameterized function symbol $\text{educated\_at}_{\text{(degree,BSc)}}(\text{AlbertEinstein}, \text{ETHZurich})$. Then, we note that $\Omega$ is a finite set, meaning that also the number of different parameterizations for the function symbol is finite, which means that this becomes a first order logic statement. In this formalism, the KG is the conjunction of all FOL statements.

In this work, we restrict the qualifiers to respect monotonicity in the KG in the following sense:

$$(h, r, t, qp) \in G \land qp' \subseteq qp \implies (h, r, t, qp') \in G$$

This implies that if a qualified statement in the KG has a set of qualifier pairs, then the KG also contains the qualified statement with any subset thereof. As a result, some types of qualifying
information cannot be used, e.g., a qualifier indicating that a relation does not hold (i.e., negation). This breaks monotonicity since the existence of such a statement would further imply the existence of that statement without the qualifier, leading to contradiction.

We define a hyper-relational query on a hyper-relational KG as follows:

**Definition 3.2** (Hyper-relational Query). Let \( \mathcal{V} \) be a set of variable symbols, and \( \text{TAR} \in \mathcal{V} \) a special variable denoting the target of the query. Let \( \mathcal{E}^+ = \mathcal{E} \cup \mathcal{V} \). Then, any subset \( Q \) of \( (\mathcal{E}^+ \times \mathcal{R} \times \mathcal{E}^+ \times \Omega) \) is a valid query if its induced graph 1) is a directed acyclic graph, 2) has a topological ordering in which all entities (in this context referred to as anchors) occur before all variables, and 3) \( \text{TAR} \) must be last in the topological orderings.

The answers \( A_Q(Q) \) to the query \( Q \) are the entities \( e \in \mathcal{E} \) that can be assigned to \( \text{TAR} \), for which there exist a variable assignment for all other variables occurring in the query graph, such that the instantiated query graph is a subgraph of the complete graph \( \mathcal{G} \).

From our definition of KG, queries, and the monotonicity requirement, we can derive that adding more qualifiers to the statements of a query can only reduce the set of possible answers to the query. The theorem and its proof can be found in the supplementary material.

In real-world KGs, information is nearly always incomplete [15]. Hence, in this work, we will answer hyper-relational queries on KGs, but in the specific setting where both entities and statements are missing from the KG.

**Problem Definition.** Given the incomplete KG \( \mathcal{G} \) (part of the not available complete KG \( \hat{\mathcal{G}} \)) and a query \( Q \). Rank all entities in \( \mathcal{G} \) such that answers to the query, if it were asked in the context of the complete KG \( \hat{\mathcal{G}} \), are at the top of the ranking.

Since the given KG is not complete, we cannot solve this problem directly as a graph matching problem as usually done in databases. Instead, we compute a latent representation of the query, such that it is close to the embeddings of entities which are the correct answers to the query.

### 4 Model Description

Our model is not trained directly on the KG, but rather with a set of queries sampled from it (see Section 5.1). Hence, to describe our model, we consider a query \( Q \subset (\mathcal{E}^+ \times \mathcal{R} \times \mathcal{E}^+ \times \Omega) \), and describe how we learn to represent it.

Our model learns representations for entities and the special symbols \( \{\text{VAR}, \text{TAR}\} \), \( \tilde{\mathcal{E}} \in \mathbb{R}^{(|\mathcal{E}|+2) \times d} \), and relation representations \( \mathcal{R} \in \mathbb{R}^{2|\mathcal{R}| \times d} \), where \( d \) is a hyper-parameter indicating the embedding dimension. There are two representations for each relation. For a statement \( s = (h, r, t, qp) \in Q \), one is used for computing “forward” messages from \( h \rightarrow t \), and the other one to compute “backward” messages from \( h \leftarrow t \). In other words, we also learn representations for the inverse relation \( r^{-1} \).

We encode the query graph using a sequence of \( \text{StaRe} \) layers [11]. First, we select from \( \tilde{\mathcal{E}} \) the embeddings needed. These are the ones for all entities in the query, \( \text{VAR} \) if the query has internal variables, and \( \text{TAR} \). These are put in \( \mathcal{E} \), which has one copy of \( \text{VAR} \) for each unique variable in \( Q \).

Each layer enriches the entity and relation representations \( \mathcal{E}, \mathcal{R} \) to \( \mathcal{E}', \mathcal{R}' \) as follows: For each query statement \( s = (h, r, t, qp) \in Q \), we compute messages \( m_{h \rightarrow t, qp} \) and \( m_{h \rightarrow t, r, qp} \). For brevity, we only describe \( m_{h \rightarrow t, qp} \), the other direction works analogously. We begin by composing the representations of the components of each qualifier pair \( q_i = (qr_i, qe_i) \in Q \) into a single representation: \( h_{qi} = \gamma_q(\mathcal{E}[qr_i], \mathcal{R}[qe_i]) \), where \( \gamma_q \) denotes a composition function [26], e.g., the Hadamard product, and we use \( \mathcal{X}[y] \) to indicate the representation of \( y \) in \( \mathcal{X} \). Next, we aggregate all qualifier pair representations for \( qp \), as well as the representation of the main relation \( r \) into a qualified relation representation using an aggregation function \( \phi_r \): \( h_{r, qp} = \phi_r(\mathcal{R}[r], \{h_{qi}\})_{q_i \in qp} \). For \( \phi_r \), we experiment with a simple sum aggregation, and an attention mechanism. To obtain a message \( m_{h \rightarrow t, qp} \), the qualified relation representation is further composed with the source entity representation \( \mathcal{E}[h] \) using another composition function \( \gamma_r \). The result gets linearly transformed.

---

[1] The queries considered here are a subset of SPARQL* basic graph pattern queries.

[2] These requirements are common in the literature, and usually stated with formal logic, but not a strict requirement for our approach. See the supplement for more information.
We introduce hyper-relational variants of 7 query patterns commonly used in the related work [13, 20, 2, 24] where each edge can have 0..n qualifier pairs. The patterns contain projection queries (designated with -p), intersection queries (designated with -i), and their combinations (cf. Fig. 2). Note that the simplest 1p pattern corresponds to a well-studied link prediction task. Qualifiers enable more flexibility in query pattern construction, i.e., we further modify formulas by conditioning the existence of qualifiers and their amount over a particular edge. We include dataset statistics and further details as to dataset construction in the supplementary material.

These formulas are then translated to the SPARQL* format [14] and used to retrieve materialized query graphs from specific graph splits. Following existing work, we make sure that validation and test queries contain at least one edge unseen in the training queries, such that evaluated models have to predict new links in addition to query answering. As we are in the transductive setup where all

Figure 2: The hyper-relational formulas and their graphical structures. The qualifier pairs attached to each edge may vary in 0..n; for visualization purposes we represent them as a single pair. We also allow qualifiers to exist only on certain edges of a query, i.e., not all edges necessarily contain them.

by $W_{e\rightarrow}$, a layer specific trainable parameter: $m_{h\rightarrow t,r,qp} = W_{e\rightarrow} \gamma_r (E[h], h_{r,qp})$. Inverse relations use a separate weight $W_{e\leftarrow}$. Next, we aggregate all incoming messages $a_e = \phi_m (m_{h\rightarrow t',r,qp} \mid (h,r,t',qp) \in Q, t = t')$ using a message aggregation function $\phi_m$, e.g., a (weighted) sum. Besides computing these message aggregates in each direction, we also compute a self-loop update $a_e = W_{e\rightarrow} \phi_r (e, r, c)$, where $W_{e\rightarrow}, r$ are trainable parameters. The updated entity representation is then obtained as the average over both directions and the self loop, with an additional activation $\sigma$ applied to it: $E'[e] = \sigma (\frac{1}{2} (a_e + a_e + a_{e,-}))$ Finally, the relation representations are updated by a linear transformation $R[r] = W_r R[r]$, where $W_r$ is a layer specific trainable weight.

After applying multiple STAR*E layers, we obtain enriched node representations $E^*$ for all nodes in the query graph. As final query representation $x_Q$, we aggregate all node representations of the query graph, $x_Q = \phi_q (E^*[e] \mid e \in E^* \land ((e,r,t,qp) \in Q \lor (h,r,e,qp) \in Q))$, with $\phi_q$ denoting an aggregation function, e.g., the sum. Alternatively, we only select the final representation of the unique target node, $x_Q = E^*[Q,T,A]$. To score answer entity candidates, we use the similarity of the query representation and the entity representation, i.e., $score(Q,e) = sim(x_Q, E^*[e])$, for a simple vector similarity function, such as the dot product, or cosine similarity.

We designate the described model as STARQE (Query Embedding for RDF Star Graphs) since RDF* is one of the most widely adopted standards for hyper-relational KGs.

5 Experiments

In this section, we empirically evaluate the performance of query answering over hyper-relational KGs. We design experiments to tackle the following research questions: RQ1) Does query answering performance benefit from qualifiers? RQ2) What are the generalization capabilities of hyper-relational query answering? RQ3) Does query answering performance depend on the physical representation of a hyper-relational KG, i.e., reification?

5.1 Dataset

Existing QE datasets based on Freebase [25] and NELL [7] are not applicable in our case since their underlying KGs are strictly triple-based. Thus, we design a new hyper-relational QE dataset based on WD50K [11] comprised of Wikidata statements, with varying numbers of qualifiers.

WD50K QE. We introduce hyper-relational variants of 7 query patterns commonly used in the related work [13, 20, 2, 24] where each edge can have 0..n qualifier pairs. The patterns contain projection queries (designated with -p), intersection queries (designated with -i), and their combinations (cf. Fig. 2). Note that the simplest 1p pattern corresponds to a well-studied link prediction task. Qualifiers enable more flexibility in query pattern construction, i.e., we further modify formulas by conditioning the existence of qualifiers and their amount over a particular edge. We include dataset statistics and further details as to dataset construction in the supplementary material.

These formulas are then translated to the SPARQL* format [14] and used to retrieve materialized query graphs from specific graph splits. Following existing work, we make sure that validation and test queries contain at least one edge unseen in the training queries, such that evaluated models have to predict new links in addition to query answering. As we are in the transductive setup where all

This dataset is available under CC BY 4.0.
Figure 3: Example of a reification process: An original hr-2p query pattern (left) is reified by the means of standard RDF reification (right). Note the change of the graph topology: the reified variant has two auxiliary nodes, three new pre-defined relation types, and original edge types became nodes connected via the `rdf:predicate` edge. The distance between the anchor and target increased, too.

entities and relation types have to be seen in training, we also ensure this for all entity and relation types appearing in qualifiers.

Due to the (current) lack of standardized data storage format for hyper-relational (RDF*) graphs in graph databases, particular implementations of RDF* employ reification, i.e., transformation of hyper-relational statements as defined in Section 3 to plain triples. Reification approaches introduce auxiliary virtual nodes, new relation types, turn relations into nodes, and might dramatically change the original graph topology. An example of a standard RDF reification in Fig. 3 transforms an original hr-2p query with three nodes, two edges, and two qualifier pairs into a new graph with nine nodes and eight edges with rigidly defined edge types.

However, the logical interpretation of a query remains the same. Therefore, we want hyper-relational QE models to be robust to the underlying graph topology. For this reason, we ship dataset queries in both formats, i.e., hyper-relational RDF* and reified with triples, and study the performance difference in a dedicated experiment.

5.2 Evaluation Protocol

In all experiments, we evaluate the model in the rank-based evaluation setting. Each query is encoded into a query embedding vector $x_q \in \mathbb{R}$. We compute a similarity score $\text{sim}(x_q, E[e])$ between the query embedding and the entity representation for each entity $e \in E$. The rank $r \in \mathbb{N}^+$ of an entity is its position in the list of entities sorted decreasingly by score. We compute filtered ranks [5], i.e., while computing the rank of a correct entity, we ignore the scores of other correct entities. We resolve exactly equal scores using the realistic rank [4], i.e., all entities with equal score obtain the rank of the average of the first and last position.

Given a set of individual ranks $\{r_i\}_{i=1}^n$, we aggregate them into a single-figure measure using several different aggregation measures: The Hits@k (H@k) metric measures the frequency of ranks at most $k \in \mathbb{N}^+$, i.e., $H@k = \frac{1}{n} \sum \mathbb{I}[r_i \leq k]$, with $\mathbb{I}$ denoting the indicator function. H@k lies between zero and one, with larger values showing better performance. The Mean Reciprocal Rank (MRR) is the (arithmetic) mean over the reciprocal ranks, i.e., $\text{MRR} = \frac{1}{n} \sum r_i^{-1}$, with a value range of $(0, 1]$, and larger values indicating better results. It can be equivalently interpreted as the inverse harmonic mean over all ranks, and thus is strongly influenced by smaller ranks.

Since the size of the answer set of queries varies greatly, queries with large answer sets would strongly influence the overall score compared to very specific queries with a single entity as answer. In contrast to rank-based evaluation in existing QE work, we propose to weight each rank in the aforementioned averages by the inverse cardinality of the answer set to compensate for their imbalance. Thereby, each query contributes an equal proportion to the final score.

---

For, e.g., hr-2p we observe a maximum answer set cardinality of 1,351, while the upper quartile is only 3.
Table 1: Query answering performance of STARQE and the baselines when training on all hyper-relational query patterns. We omit the hr- prefix for brevity.

| Pattern | 1p | 2p | 3p | 2i | 3i | 2i-1p | 1p-2i |
|---------|----|----|----|----|----|-------|-------|
| Hits@10 (%) |
| StarQE   | 51.72 | 51.20 | 65.50 | 77.78 | 92.64 | 61.81 | 81.60 |
| Base Triple | 45.04 | 12.76 | 24.66 | 69.74 | 91.74 | 16.77 | 40.67 |
| Reification | 55.17 | 50.86 | 63.65 | 81.25 | 95.31 | 61.05 | 80.49 |
| Zero Layers | 44.93 | 29.94 | 38.45 | 67.79 | 90.66 | 35.48 | 47.85 |
| MRR (%) |
| StarQE   | 30.98 | 44.13 | 52.96 | 63.14 | 83.78 | 55.20 | 71.52 |
| Base Triple | 22.25 | 6.73 | 14.05 | 48.01 | 74.52 | 8.16 | 22.23 |
| Reification | 34.78 | 43.42 | 50.77 | 61.01 | 85.17 | 49.09 | 64.21 |
| Zero Layers | 27.55 | 19.10 | 21.25 | 50.27 | 80.62 | 24.49 | 30.04 |

5.3 Hyper-relational Query Answering

As we are the first to introduce the problem of hyper-relational query answering, there is no established baseline available at the time of writing. Hence, we compare our method to several strong baselines.

Implementation. We implement STARQE and other baselines in PyTorch (MIT License). We run a hyperparameter optimization (HPO) pipeline on a validation set for each model and report the best setup in the supplementary materials. All experiments are run on single NVidia GTX 1080 Ti or RTX 2080 Ti GPU. The machines in the internal clusters had between 12 and 32 CPUs, but these and the main memory had low utilization rates.

Base Triple. For the first baseline, we thoroughly remove all qualifiers from the hyper-relational statements in the query graph keeping just the base triples (h, r, t). Thus, we can investigate whether it is vital to consider the additional signal of qualifiers to answer the queries correctly or whether the bare triples are already sufficient. Notice that we still use the exact same query graphs as in other experiments, but remove the qualifiers upon loading. The set of targets for these queries remains unchanged, e.g., having a hyper-relational query from Fig. we drop the (degree: BSc) qualifier but still have only ETHZürich as a correct answer. Otherwise, the triple-only queries that often have more correct answers would make the results incomparable.

Reification. For the second setting, we convert the hyper-relational query graph to plain triples via reification as described in Section 5.1. Here, we investigate whether STARQE is able to produce the same semantic interpretation of a topologically different query. Note that, while conceptually the default relation enrichment mechanism of STARQE resembles singleton property reification, its semantic interpretation is equivalent to standard RDF reification.

Zero Layers. As an additional baseline, we consider a model akin to bag-of-words, which trains entity and relation embeddings but does not employ any message passing step before graph aggregation.

Discussion.

The results shown in Table indicate that STARQE, in general, is able to tackle hyper-relational queries of varying complexity. That is, the performance on complex intersection and projection queries is often higher than that of a simple link prediction (hr-1p). Particularly, queries with intersections (¬i) demonstrate outstanding accuracy. Importantly, MRR values are relatively close to Hits@10 which means that more precise measures like Hits@3 and Hits@1 retain good performance (we provide a detailed breakdown in the supplementary materials).

To investigate if this performance could be attributed to the impact of qualifiers, we run a Base Triple baseline. The results suggest that qualifiers play an especially important role in projection (¬p) queries as the performance gaps reach, e.g., more than 40 Hits@10 points on 3p queries. We hypothesize this can be explained by the fact that qualifiers also effectively reduce the size of intermediate variable answers, and our qualifier-aware encoder can capture that.

https://github.com/DimitrisAlivas/StarQE
We observe a comparative performance running the Reification baseline. It suggests that our QE framework is robust to the underlying graph topology retaining the same logical interpretation of a complex query. We believe it is a promising sign of enabling hyper-relational query answering on a wide range of physical graph implementations.

Finally, we find that message passing layers are essential for maintaining high accuracy as the Zero Layers baseline lags far behind GNN-enabled models. One explanation for this observation can be that without message passing variable nodes do not receive any updates and are thus not “resolved” properly. To some extent counter-intuitively, we also observed that it does not make a large difference whether relation embeddings are included in the aggregation or not. Relatively high performance on 1p, 2i, 3i queries can be explained by their very specific star-shaped query pattern which is essentially 1-hop with multiple branches joining at the center node.

### 5.4 Generalization

Following the related work, we experiment with how well our approach can generalize to complex query patterns if trained on simple ones. Note that below we understand all query patterns as hyper-relational, i.e., having the hr- prefix. There exist several styles for measuring generalization in the literature that we include in the experiment:

**Q2B-like.** The style is used by QUERY2Box [20] and assumes training only on 1p, 2p, 3p, 2i, 3i queries while evaluating on two additional patterns 2i-1p, 1p-2i.

**EmQL-like.** The other approach proposed by EmQL [24] employs only 1p, 2i patterns for training, using five more complex ones for evaluation.

**MPQE-like.** The hardest generalization setup used in MPQE [8] allows training only on 1p queries, i.e., vanilla link prediction, while all evaluation queries include unseen intersections and projections.

**MPQE-like + Reif.** To measure the impact of reification on generalization, we also run the experiment on reified versions of all query patterns. Similarly to MPQE-like, this setup allows training only on 1p reified pattern and evaluates the performance on other, more complex reified patterns.

**Discussion.**

Table 2 summarizes the generalization results. As a reference point, we include the StarQE results in the no-generalization setup when training and evaluating on all query patterns. Generally, we observe that all setups generalise well on intersection queries (-i) even when training in the most restricted (1p) mode. The Q2B-like regime demonstrates appealing generalization capabilities on (2i-1p, 2p-1i), indicating that it is not necessary to train QE models on all available query types. Going to a fine-grained study of most impactful patterns, we, however, find that projection (-p)
patterns are rather important for generalization, as both *emQL* and *MPQE* styles dramatically fall behind in accuracy, especially in the MRR metric which indicates that higher precision results are impaired the most.

The *MPQE* style is clearly the hardest when having only one training pattern. The higher results on intersection (-i) patterns can be explained by a small cardinality of the answer set, i.e., qualifiers make a query very selective with very few possible answers. Finally, it appears that reification (*MPQE+ Reif*) impedes generalization capabilities and overall accuracy according to the MRR results. This can be explained by sophisticated graph topologies produced when reifying complex queries, and training only on 1p is not sufficient for such complex graphs.

6 Limitations & Future Work

In this section, we discuss limitations of the current work, and future research directions. The first limitation of our work is that we do not allow literal values like numbers, text, and time in our graph. This means that we cannot, for example, handle queries asking for people born in the year 1980. A future investigation could consider such values, and seemingly it should be possible to incorporate these into GNN models as node features.

Secondly, our work assumes monotonicity of the qualifiers. Working without this assumption is an interesting future direction. Thirdly, there are several other logical operators we could include. Not only negation (which could be included as a qualifier), but also disjunctions, cardinality constraints, etc. Another interesting next step is to allow for variables in more positions of the query. In this work, we only allow variables in the head and tail positions. Nonetheless, one can also formulate more general graph queries with variables in the qualifier value, and even in the relation position.

Moreover, the current work already allows for different query shapes compared to prior work because queries are not limited to DAGs (see supplementary materials for details). However, our work does not allow all shapes. Specifically, it is currently unclear how queries with cycles would behave. Besides, we also noticed, similar to other works, that queries with many hops are harder. This appears to be a similar issue to grasping long-range dependencies in sequences, and further investigation in this direction is required.

One more aspect to be looked at are the many operators and possibilities which query languages like SPARQL have. For example, queries including paths, aggregations, sub-queries, filters on literals, etc. Further research work is also needed in the domain of explainability. The system does currently produce an answer without providing an explanation. One potential solution is to not only look for the target of the query, but also provide answers for the intermediate variables.

A final interesting research direction is the use of approximate query answering for the creation of query plans. If an set of likely correct answers can be determined fast, this information could be used to choose a more optimal plan for exact query execution.

7 Conclusion

In this work, we have studied and addressed the extension of the multi-hop logical reasoning problem to hyper-relational KGs. We touched upon the theoretical considerations of having qualifiers in the context of query answering and discussed the effects it can have on query answering such as cardinality of the answer set. We also proposed the first hyper-relational QE model, STARQE, based on a Graph Neural Network encoder to work in this new setup. Further, we introduced a new dataset, WD50K QE, with hyper-relational variants of 7 well studied query patterns and analysed the performance of our models on each of them individually and on average. Our results suggest that qualifiers indeed help to obtain more accurate answers compared to triple-only graphs. We also demonstrate the robustness of our approach to particular concrete implementations of hyper-relational graphs in graph databases that often involve reification. Finally, we evaluate generalisation capabilities of our model in various settings and find that it is able to accurately answer unseen patterns.

Potential negative societal impacts of this work. As with all technologies that attempt to derive new information from existing one, there could be both negative and positive impacts of the technology. For example, approximate query answering could be used for drug re-purposing, but it could, in principle, also be used by an oppressive government to predict information about people.
A further issue is the assumption of this and related techniques that the data used for training only contains true facts. If this data is (intentionally) biased or erroneous to start with, further biased or wrong information will be derived, which could lead to harmful conclusions and decisions. Besides, even if the input data to the system is correct, the system could due to its imperfections still derive incorrect answers to queries, which might, again lead to wrong conclusions. Hence, users of this technology must be made aware that answers to their queries are always approximate, and this technology ought not to be used in a process where correctness is critical.

References

[1] M. Ali, M. Berrendorf, C. T. Hoyt, L. Vermue, M. Galkin, S. Sharifzadeh, A. Fischer, V. Tresp, and J. Lehmann. Bringing light into the dark: A large-scale evaluation of knowledge graph embedding models under a unified framework. CoRR, abs/2006.13365, 2020.

[2] E. Arakelyan, D. Daza, P. Minervini, and M. Cochez. Complex query answering with neural link predictors. In International Conference on Learning Representations, 2021. URL https://openreview.net/forum?id=Mos9F9kDwkz

[3] C. Berge. Hypergraphs: combinatorics of finite sets, volume 45. Elsevier, 1984.

[4] M. Berrendorf, E. Faerman, L. Vermue, and V. Tresp. Interpretable and fair comparison of link prediction or entity alignment methods with adjusted mean rank. CoRR, abs/2002.06914, 2020. URL https://arxiv.org/abs/2002.06914

[5] A. Bordes, N. Usunier, A. García-Durán, J. Weston, and O. Yakhnenko. Translating embeddings for modeling multi-relational data. In C. J. C. Burges, L. Bottou, Z. Ghahramani, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 26: 27th Annual Conference on Neural Information Processing Systems 2013. Proceedings of a meeting held December 5-8, 2013, Lake Tahoe, Nevada, United States, pages 2787–2795, 2013.

[6] D. Brickley, R. V. Guha, and B. McBride. RDF schema 1.1. W3C recommendation, 25: 2004–2014, 2014.

[7] A. Carlson, J. Betteridge, B. Kisiel, B. Settles, E. R. H. Jr., and T. M. Mitchell. Toward an architecture for never-ending language learning. In M. Fox and D. Poole, editors, Proceedings of the Twenty-Fourth AAAI Conference on Artificial Intelligence, AAAI 2010, Atlanta, Georgia, USA, July 11-15, 2010. AAAI Press, 2010.

[8] D. Daza and M. Cochez. Message passing query embedding. In ICML Workshop - Graph Representation Learning and Beyond, 2020. URL https://arxiv.org/abs/2002.02406

[9] F. Erxleben, M. Günther, M. Krützsch, J. Mendez, and D. Vrandecic. Introducing wikidata to the linked data web. In P. Mika, T. Tudorache, A. Bernstein, C. Welty, C. A. Knoblock, D. Vrandecic, P. Groth, N. F. Noy, K. Janowicz, and C. A. Goble, editors, The Semantic Web - ISWC 2014 - 13th International Semantic Web Conference, Riva del Garda, Italy, October 19-23, 2014. Proceedings, Part I, volume 8796 of Lecture Notes in Computer Science, pages 50–65. Springer, 2014. doi: 10.1007/978-3-319-11964-9_4. URL https://doi.org/10.1007/978-3-319-11964-9_4

[10] J. Frey, K. Müller, S. Hellmann, E. Rahm, and M. Vidal. Evaluation of metadata representations in RDF stores. Semantic Web, 10(2):205–229, 2019.

[11] M. Galkin, P. Trivedi, G. Maheshwari, R. Usbeck, and J. Lehmann. Message passing for hyper-relational knowledge graphs. In B. Webber, T. Cohn, Y. He, and Y. Liu, editors, Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing, EMNLP 2020, Online, November 16-20, 2020, pages 7346–7359. Association for Computational Linguistics, 2020.

[12] S. Guan, X. Jin, J. Guo, Y. Wang, and X. Cheng. Neuinfer: Knowledge inference on n-ary facts. In Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics, pages 6141–6151, 2020.
[13] W. L. Hamilton, P. Bajaj, M. Zitnik, D. Jurafsky, and J. Leskovec. Embedding logical queries on knowledge graphs. In S. Bengio, H. M. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada, pages 2030–2041, 2018.

[14] O. Hartig. Foundations of RDF*: and SPARQL*: (an alternative approach to statement-level metadata in RDF). In AMW 2017 11th Alberto Mendelzon International Workshop on Foundations of Data Management and the Web, Montevideo, Uruguay, June 7-9, 2017., volume 1912. Juan Reutter, Divesh Srivastava, 2017.

[15] A. Hogan, E. Blomqvist, M. Cochez, C. d’Amato, G. de Melo, C. Gutierrez, J. E. L. Gayo, S. Kirrane, S. Neumaier, A. Polleres, R. Navigli, A.-C. N. Ngomo, S. M. Rashid, A. Rula, L. Schmelzeisen, J. Sequeda, S. Staab, and A. Zimmermann. Knowledge graphs, 2021.

[16] S. Ji, S. Pan, E. Cambria, P. Marttinen, and P. S. Yu. A survey on knowledge graphs: Representation, acquisition and applications. CoRR, abs/2002.00388, 2020.

[17] B. Kotnis, C. Lawrence, and M. Niepert. Answering complex queries in knowledge graphs with bidirectional sequence encoders. CoRR, abs/2004.02596, 2020.

[18] A. Paszke, S. Gross, F. Massa, A. Lerer, J. Bradbury, G. Chanan, T. Killeen, Z. Lin, N. Gimelshein, L. Antiga, A. Desmaison, A. Köpf, E. Yang, Z. DeVito, M. Raison, A. Tejani, S. Chilamkurthy, B. Steiner, L. Fang, J. Bai, and S. Chintala. Pytorch: An imperative style, high-performance deep learning library. In Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada, pages 8024–8035, 2019.

[19] H. Ren and J. Leskovec. Beta embeddings for multi-hop logical reasoning in knowledge graphs. In H. Larochelle, M. Ranzato, R. Hadsell, M. Balcan, and H. Lin, editors, Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual, 2020.

[20] H. Ren, W. Hu, and J. Leskovec. Query2box: Reasoning over knowledge graphs in vector space using box embeddings. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020. OpenReview.net, 2020. URL https://openreview.net/forum?id=BJgr4kSFDS.

[21] P. Rosso, D. Yang, and P. Cudré-Mauroux. Beyond triplets: hyper-relational knowledge graph embedding for link prediction. In Proceedings of The Web Conference 2020, pages 1885–1896, 2020.

[22] M. Schlichtkrull, T. N. Kipf, P. Bloem, R. Van Den Berg, I. Titov, and M. Welling. Modeling relational data with graph convolutional networks. In European semantic web conference, pages 593–607. Springer, 2018.

[23] F. M. Suchanek, G. Kasneci, and G. Weikum. Yago: a core of semantic knowledge. In Proceedings of the 16th international conference on World Wide Web, pages 697–706, 2007.

[24] H. Sun, A. O. Arnold, T. Bedrax-Weiss, F. Pereira, and W. W. Cohen. Faithful embeddings for knowledge base queries. In H. Larochelle, M. Ranzato, R. Hadsell, M. Balcan, and H. Lin, editors, Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual, 2020.

[25] K. Toutanova and D. Chen. Observed versus latent features for knowledge base and text inference. In Proceedings of the 3rd Workshop on Continuous Vector Space Models and their Compositionality, pages 57–66, Beijing, China, July 2015. Association for Computational Linguistics. doi: 10.18653/v1/W15-4007. URL https://www.aclweb.org/anthology/W15-4007.

[26] S. Vashishth, S. Sanyal, V. Nitin, and P. P. Talukdar. Composition-based multi-relational graph convolutional networks. In 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020. OpenReview.net, 2020.
[27] A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, L. Kaiser, and I. Polosukhin. Attention is all you need. In I. Guyon, U. von Luxburg, S. Bengio, H. M. Wallach, R. Fergus, S. V. N. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA, pages 5998–6008, 2017.

[28] P. Veličković, G. Cucurull, A. Casanova, A. Romero, P. Liò, and Y. Bengio. Graph attention networks. In International Conference on Learning Representations, 2018. URL https://openreview.net/forum?id=rJXMpikCZ.

[29] D. Vrandečić and M. Krötzsch. Wikidata: a free collaborative knowledgebase. Communications of the ACM, 57(10):78–85, 2014.

[30] W. X. Wilcke, P. Bloem, V. de Boer, R. H. van t Veer, and F. A. H. van Harmelen. End-to-end entity classification on multimodal knowledge graphs, 2020.

[31] M. Zaheer, S. Kottur, S. Ravanbakhsh, B. Poczos, R. R. Salakhutdinov, and A. J. Smola. Deep sets. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems 30, pages 3391–3401. Curran Associates, Inc., 2017. URL http://papers.nips.cc/paper/6931-deep-sets.pdf.
Appendix

A Types of Graphs

In this section, we discuss in further detail the different approaches to break free from the restriction of pairwise relations. The intuition how those approaches are different is presented in Fig. 4.

Hyper-relational Graphs KGs used in our work are a subset of hyper-relational graphs. In general, hyper-relational graphs can also contain literal values, like integers and string values as qualifier values. Labeled property graphs are another example of a subset of hyper-relation graphs, but they typically only allow literals as qualifier values. The Wikidata model [9] and RDF* [14] allows for both literals and entities as values. Many implementations of RDF* do make the monotonicity assumption, which we also made in the paper. Some will also merge statements in case they have the same main triple. The resulting statement will have the same main triple, but as qualifier information, the union of the sets of qualifier pairs of the original statements.

Hypergraphs Hypergraphs are another type of graphs, initially proposed by Berge [3], where hyperedges link one or more vertices. These hyperedges group together sets of nodes in a relation, but lose information of the particular roles that entities play in this relation. Besides, each different composition of elements in the relation introduces a new hyperedge type, causing a combinatorial explosion of these types.

Reified Graphs Hyper-relational and reified graphs have equivalent expressive power compared to labelled directed graphs. The reason is that we can define a bijection between these graphs. However, depending on the use case, the different graph types have benefits. When we convert a hyper-relational graph to an RDF graph, we end up with what is called the reified graph. There are multiple approaches on how to perform this conversion. In our work, we use Standard RDF Reification[9] It introduces new, so called blank nodes to represent statements with all parts of a statement attached. This allows for all information to exist on the same level. One of the disadvantages to this approach is the addition of auxiliary nodes, which heavily affect the structure of the graph and quickly inflate the graph size.

B The WD50K-QE Dataset

In this section, we describe the processes of generating the hyper-relational query samples that we use for training, validating and testing our models. To sample our queries, our data are hosted on a graph database with support for hyper-relational data. For our use-case, we use anzograph[10]. WD50K [11] is a dataset created to counter the flaws of other hyper-relational datasets. It is publicly available by the authors, in CSV format. In order to utilise it for our work, we started by converting the dataset from CSV to RDF*.

In order to generate the query data splits, we constructed SPARQL* queries that correspond to a specific pattern. Using a query language to generate query samples has certain advantages and disadvantages over other approaches found in the related work. In the related work, we encounter sampling using different techniques such as random walks, often after the removal of a certain percentage of edges. With our approach, we have more control over what the samples will look like, and thus a finer control of the inputs to our experiments. Moreover, we can also ensure that we do not sample with replacement and at the same time make sure we do not sample queries that are isomorphic with each other. A final benefit is that with our approach, we can immediately get all answers for a query, instead of only one. We utilized named graphs[11] in order to keep our train, validation and test triples disconnected, therefore ensuring no data leakage. In the evaluation of approximate query answering, it is common to have queries with at least one unseen edge from

https://www.w3.org/TR/2014/REC-rdf11-mt-20140225/#reification
https://www.cambridgesemantics.com/anzograph/
https://www.w3.org/TR/rdf11-concepts/#section-dataset
the test set. As such, and given the edges of the graph, we split them in 3 corresponding to the aforementioned named graphs as: \textit{triple\_train}, \textit{triple\_validation}, and \textit{triple\_test}.

Based on these we create the train, validation, and test sets for our approximate query answering dataset with the following assumptions:

- For the training set, all triples come from the \textit{triple\_train} set (only).
- For the validation set, one triple comes from the \textit{triple\_validation} and the other edge(s) come from either \textit{triple\_train} or \textit{triple\_validation}, and
- For the test set, one triple comes from \textit{triple\_test}, and the other triple from any of \textit{triple\_train}, \textit{triple\_validation}, and \textit{triple\_test}

One final issue we encountered had to do with the nodes with a high in degree in our dataset. Their existence causes a skewing of the distribution of correct answers to queries, and has to be resolved. In Appendix C we refer to this issue and explain our approach.

C Issues Sampling Queries with Joins in a Graph with High Degree Nodes

In our query generation step, we exclude high in-degree nodes as a target for specific queries. In this section, we explain why that choice was made. We will focus on the \textit{3i} pattern. The same argument holds for other patterns with joins, like \textit{2i}, \textit{2i-1p}, \textit{1p-2i}.

The queries are randomly sampled from all possible queries that can be formed by matching the pattern with the data graph. For the \textit{3i} pattern, a node with an in-degree of \(n\), results in \(\binom{n}{3}\) different queries, with that node as a target.

The problem is that if we randomly sample our queries, the answer would usually be one of the highest degree nodes. Concretely, in our graph data, the highest observed in-degree is 4,424, which would result in 14,421,138,424 possible queries with the corresponding node as an answer. If we generated all possible queries, we would end up with 38,011,148,464 different ones. So, the node with the highest in-degree is already responsible for 38\% of the queries, meaning that system answering 3-i queries that are randomly sampled, would get 38\% correct by always giving that answer. Moreover, if we look at the Hits@10 metric, we would score 93\%, by always predicting the same ranking (the top 10 in descending frequency). Note that existing query embedding models have been evaluated like this in the past, ignoring this data issue.

Hence, we decided to make the task harder by removing these high degree nodes for queries with joins. That is, by putting the threshold at an in-degree of 50, we remove the 623 nodes with the highest in-degree which would have represented 99.9\% of the possible answers for the \textit{3i} queries without this modification. After filtering, the baseline of always predicting the same ranking for the randomly sampled queries, will result in a Hits@10 of 3\% in the best case.
Figure 5: A diagram of the query generation process. On the far left, the chosen dataset (WD50K) is uploaded in the RDF*-compatible triplestore (AnzoGraph). As a follow up, we translated the hyper-relational query patterns to SPARQL* and executed them against the triplestore to retrieve the desired splits.

For other query shapes where a join is involved, the situation is similar, but less pronounced.

D Size of the Answer Set of a Query with more Qualifiers

When we have a query with or without qualifiers, and we add more qualifiers, the number of answers to this query can only become smaller. Intuitively, this happens because the query becomes more specific. In this section we prove this intuition correct. Note that proving this requires monotonicity, as we defined in the paper. Without this assumption - for example allowing non-monotonic qualifier relations - would result in losing the guarantee that the answer set becomes smaller.

Given a query $Q$, and a query $\overline{Q}$ that is the same, except for one set of qualifier pairs of $Q$ which can have extra pairs, then the answers to $\overline{Q}$ are a subset of the answers to $Q$.

Formally:

**Theorem D.1.** Given a KG $\mathcal{G} = (E, R, S)$, where $S \subseteq (E \times R \times E \times \Omega)$, a query $Q = \{(h_1, r_1, t_1, q_{p_1}), \ldots, (h_n, r_n, t_n, q_{p_n})\}$, and a second query $\overline{Q} = \{(h_1, r_1, t_1, q'_{p_1}), \ldots, (h_n, r_n, t_n, q'_{p_n})\}$, where $\exists! k : q_{p_k} \subseteq q'_{p_k}$ and $\forall x((x \in [1, \ldots n] \land x \neq k) \rightarrow q_{p_x} = q'_{p_x})$. Then, $A_{\mathcal{G}}(\overline{Q}) \subseteq A_{\mathcal{G}}(Q)$.

**Proof.** Assuming symbols as defined in the theorem, we show that $\forall a : a \in A_{\mathcal{G}}(\overline{Q}) \implies a \in A_{\mathcal{G}}(Q)$. If $a$ is an answer to $\overline{Q}$, then its associated variable substitution $v$ is such that $(v(h_k), r_k, v(t_k), q_{p_k}) \in \mathcal{G}$. From monotonicity, and given $q_{p_k} \subseteq q'_{p_k}$ we then know that $(v(h_k), r_k, v(t_k), q_{p_k}) \in \mathcal{G}$. And hence, using the same variable substitution, $a$ is an answer for $Q$. \hfill $\Box$

**Corollary D.1.** By induction, given a query $Q$, and a query $\overline{Q}$ that is the same, except for any set of qualifier pairs of $Q$ which can have extra pairs, then the answers to $\overline{Q}$ are a subset of the answers to $Q$.

**Corollary D.2.** As a special case, given a query $Q$, and a query $\overline{Q}$ that is the same, except that $Q$ does not have qualifiers, while $\overline{Q}$ can have qualifier pairs on its statements, then the answers to $\overline{Q}$ are a subset of the answers to $Q$.

\footnote{$(h, r, t, qp) \in \mathcal{G} \land qp' \subseteq qp \implies (h, r, t, qp') \in \mathcal{G}$}
E Relaxing the Requirements on Queries

In the paper, we limited our queries with the same limitations as is done in prior work. Here we will discuss why not all of these restrictions are not needed for our work, and how our evaluation already includes some of these more general cases.

As a reminder the definition of our queries is as follows:

**Definition E.1 (Hyper-relational Query).** Let $\mathcal{V}$ be a set of variable symbols, and $\text{TAR} \in \mathcal{V}$ a special variable denoting the target of the query. Let $\mathcal{E}^+ = \mathcal{E} \cup \mathcal{V}$. Then, any subset $Q$ of $(\mathcal{E}^+ \times \mathcal{R} \times \mathcal{E}^+ \times \Omega)$ is a valid query if its induced graph

1) is a directed acyclic graph,

2) has a topological ordering in which all entities (in this context referred to as anchors) occur before all variables, and

3) $\text{TAR}$ must be last in the topological orderings.

The main reason why we deal with more general queries is because our query encoder learns representation for both normal and inverse relations. We use $r^{-1}$ to indicate the inverse of relation $r$. When encoding a query with a (normal) relation $r$, then both representations $R[r]$ and $R[r^{-1}]$ are used simultaneously. If we encounter a query using the inverse relation $r^{-1}$, we can use that inverse relation $R[r^{-1}]$ and the inverse of the inverse $R[(r^{-1})^{-1}] = R[r]$, or in other words the normal relation representation of $r$. This means that even if we only ever train with the normal relation, we have the ability to invert relations, and hence we can lift some limitations.

For example, let us look at the query $Q_{\text{new\_pattern}} = \{ (e_1, r_1, \text{TAR}, \{\}), (\text{TAR}, r_2, \text{VAR}_1, \{\}), (\text{VAR}_1, r_3, e_3, \{\}) \}$. This query breaks two of the requirements. It has an entity $e_3$ occurring after variables $\text{VAR}_1$ and $\text{TAR}$ in the topological ordering. And, $\text{TAR}$ is not in the last position.

However, using inverse relations, we can convert this query into: $Q_{\text{known\_pattern}} = \{ (e_1, r_1, \text{TAR}, \{\}), (\text{VAR}_1, r_2^{-1}, \text{TAR}, \{\}), (e_3, r_3^{-1}, \text{VAR}_1, \{\}) \}$. This transformation converts the query into a 1p–2i query, which is a pattern among the evaluated patterns in the paper. Because of this transformation, the pattern of $Q_{\text{new\_pattern}}$ is indistinguishable from the pattern of $Q_{\text{known\_pattern}}$ from the perspective of the model. Besides the example illustrated above, many other graphs can be converted into one of the patterns in the paper. Since we can perform the conversion in both directions, all these possible patterns are also implicitly included in our used datasets.

In principle, the encoder does also not assume that there are no cycles in the query graph. However, the effect of cycles requires further investigation.

F Number of Message Passing Steps Equal to the Diameter

In Daza and Cochez [8], the authors find that the best results are achieved when making the number of message passing steps equal to the diameter of the query, defined as the longest shortest path between 2 nodes in it. After these steps, they use the embedding of the target variable as the embedding of the complete graph. Accordingly, we performed additional experiments with this dynamic query embedding setting, and with a variant which uses an extra message passing step. From these experiments we concluded that this approach did not lead to better results, which contradicts with the findings in [8].

G Detailed Results

We provide our chosen hyper-parameters after performing hyper-parameter optimisation in table and detailed results including standard deviation across five runs with different random seeds in Tables 4 and 5. We report Hits@k for $k = 1, 3, 10$, mean reciprocal rank (MRR), and adjusted mean rank index (AMRI) [4]. For all metrics, larger values indicate better performance. We highlight the best result per column and metric in bold font.
| Experiment       | STARQE | Base Triple | Reification | Zero Layers | MPQE-like | MPQE-like + Reif | EMQL-like | Q2B-like |
|------------------|--------|-------------|-------------|-------------|-----------|-----------------|-----------|----------|
| activation       | leakyrelu | relu       | relu        | relu        | prelu     | relu            | leakyrelu | leakyrelu |
| optimiser        | adam   | adam        | adam        | adam        | adam      | adam            | adam      | adam     |
| learning-rate    | 0.0007741 | 0.007253   | 0.003768    | 0.0008733   | 0.0005256 | 0.0001414      | 0.0007253 | 0.002075 |
| batch-size       | 64     | 32          | 32          | 64          | 128       | 32              | 128       | 32       |
| graph-pooling    | targetpooling | sum       | sum         | sum         | targetpooling | targetpooling | targetpooling | sum       |
| message-weighting| attention | attention  | attention   | symmetric   | attention | symmetric      | attention | attention |
| similarity       | dotproduct | negativepowernorm | negativepowernorm | negativepowernorm | dotproduct | dotproduct      | dotproduct | negativepowernorm |
| num-layers       | 3      | 2           | 2           | 2           | 3         | 3               | 3         | 3        |
| use-bias         | True   | True        | True        | False       | False     | False          | False     | True     |
| embedding-dim    | 192    | 224         | 224         | 160         | 128       | 96             | 256       | 224      |
| dropout          | 0.5    | 0.3         | 0.3         | 0.3         | 0.5       | 0.2            | 0.3       | 0.1      |
| composition      | multiplication | multiplication | multiplication | multiplication | multiplication | multiplication | multiplication | multiplication |
Table 4: Full results for baseline experiments, including standard deviation across five runs with different random seeds. We report Hits@k for $k = 1, 3, 10$, mean reciprocal rank (MRR), and adjusted mean rank index (AMRI) [4]. For all metrics, larger values indicate better performance. We highlight the best result per column and metric in **bold font**.

| Pattern       | 1p              | 2p              | 3p              | 2i              | 3i              | 2i-1p           | 1p-2i           |
|---------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| **Hits@1 (%)**|                 |                 |                 |                 |                 |                 |                 |
| StarQE        | 20.91 ± 1.11    | **39.98 ± 0.27**| 45.85 ± 0.81    | 55.11 ± 1.26    | 78.58 ± 1.44    | **51.77 ± 0.73**| 65.77 ± 1.87    |
| Base Triple   | 11.62 ± 0.68    | 2.97 ± 0.21     | 7.57 ± 1.59     | 36.87 ± 2.22    | 64.72 ± 6.97    | 3.33 ± 0.33     | 13.00 ± 1.07    |
| Reification   | **24.26 ± 0.88**| 38.82 ± 0.41    | 42.80 ± 0.50    | 49.67 ± 1.86    | **78.93 ± 3.20**| 42.39 ± 0.68    | 55.05 ± 1.11    |
| Zero Layers   | 18.30 ± 0.31    | 12.92 ± 0.25    | 11.53 ± 0.13    | 40.35 ± 0.82    | 74.27 ± 0.32    | 18.17 ± 0.25    | 19.51 ± 0.22    |
| **Hits@3 (%)**|                 |                 |                 |                 |                 |                 |                 |
| StarQE        | 35.58 ± 0.82    | **46.41 ± 0.32**| 57.34 ± 0.58    | 67.98 ± 0.93    | 87.56 ± 0.74    | **56.89 ± 0.47**| **75.35 ± 1.02**|
| Base Triple   | 25.54 ± 0.28    | 6.38 ± 0.32     | 15.44 ± 1.56    | 53.45 ± 2.60    | 81.55 ± 4.70    | 7.40 ± 0.67     | 23.56 ± 1.49    |
| Reification   | **40.12 ± 1.37**| 45.58 ± 0.74    | 55.45 ± 0.88    | **68.31 ± 0.77**| **89.84 ± 1.90**| 51.33 ± 0.37    | 70.26 ± 0.83    |
| Zero Layers   | 31.98 ± 0.23    | 21.34 ± 0.34    | 25.24 ± 0.27    | 55.83 ± 0.42    | 85.43 ± 0.37    | 25.75 ± 0.26    | 35.67 ± 0.28    |
| **Hits@10 (%)**|                 |                 |                 |                 |                 |                 |                 |
| StarQE        | 51.72 ± 0.66    | **51.20 ± 0.44**| **65.50 ± 0.39**| 77.78 ± 0.53    | 92.64 ± 0.65    | **61.81 ± 0.37**| **81.60 ± 0.60**|
| Base Triple   | 45.04 ± 1.18    | 12.76 ± 0.92    | 24.66 ± 2.15    | 69.74 ± 1.43    | 91.74 ± 1.83    | 16.77 ± 1.44    | 40.67 ± 1.31    |
| Reification   | **55.17 ± 1.00**| 50.86 ± 0.39    | 63.65 ± 0.60    | **81.25 ± 0.45**| **95.31 ± 0.78**| 61.05 ± 0.92    | 80.49 ± 0.81    |
| Zero Layers   | 44.93 ± 0.35    | 29.94 ± 0.35    | 38.45 ± 0.18    | 67.79 ± 0.42    | 90.66 ± 0.20    | 35.48 ± 0.31    | 47.85 ± 0.43    |
| **MRR (%)**   |                 |                 |                 |                 |                 |                 |                 |
| StarQE        | 30.98 ± 0.91    | **44.13 ± 0.28**| **52.96 ± 0.61**| **63.14 ± 0.97**| 83.78 ± 1.00    | **55.20 ± 0.52**| **71.52 ± 1.37**|
| Base Triple   | 22.25 ± 0.25    | 6.73 ± 0.28     | 14.05 ± 1.72    | 48.01 ± 2.13    | 74.52 ± 5.35    | 8.16 ± 0.62     | 22.23 ± 1.21    |
| Reification   | **34.78 ± 1.07**| 43.42 ± 0.48    | 50.77 ± 0.54    | 61.01 ± 1.17    | **85.17 ± 2.33**| 49.09 ± 0.63    | 64.21 ± 0.86    |
| Zero Layers   | 27.55 ± 0.19    | 19.10 ± 0.27    | 21.25 ± 0.14    | 50.27 ± 0.57    | 80.62 ± 0.28    | 24.49 ± 0.22    | 30.04 ± 0.21    |
| **AMRI (%)**  |                 |                 |                 |                 |                 |                 |                 |
| StarQE        | 78.44 ± 1.78    | 68.11 ± 2.52    | 74.62 ± 2.94    | 93.63 ± 0.81    | 98.65 ± 0.33    | 73.14 ± 2.39    | 88.76 ± 0.61    |
| Base Triple   | 88.14 ± 0.21    | 81.25 ± 0.46    | 95.92 ± 0.11    | 99.18 ± 0.12    | 99.95 ± 0.01    | 83.44 ± 0.95    | 98.91 ± 0.11    |
| Reification   | **88.81 ± 0.47**| 86.63 ± 1.41    | **96.20 ± 0.28**| **99.24 ± 0.10**| **99.96 ± 0.01**| 85.46 ± 0.82    | **99.10 ± 0.12**|
| Zero Layers   | 88.03 ± 0.22    | **90.56 ± 0.47**| 95.79 ± 0.20    | 96.34 ± 0.30    | 98.37 ± 0.13    | **86.18 ± 0.60**| 98.55 ± 0.10    |
Table 5: Full results for the generalization experiments, including standard deviation across five runs with different random seeds. We report Hits@k for k = 1, 3, 10, mean reciprocal rank (MRR), and adjusted mean rank index (AMRI) [4]. For all metrics, larger values indicate better performance. We highlight the best result per column and metric in **bold font**.

| Pattern                      | 1p         | 2p         | 3p         | 2i         | 3i         | 2i-1p      | 1p-2i      |
|------------------------------|------------|------------|------------|------------|------------|------------|------------|
| **Hits@1 (%)**               |            |            |            |            |            |            |            |
| StarE-like                   | 20.91 ± 1.11 | 39.98 ± 0.27 | 45.85 ± 0.81 | 55.11 ± 1.26 | 78.58 ± 1.44 | 51.77 ± 0.73 | 65.77 ± 1.87 |
| Q2B-like                     | 21.63 ± 0.70 | 37.15 ± 0.65 | 43.82 ± 0.98 | 52.49 ± 1.45 | 77.36 ± 1.46 | 37.59 ± 2.88 | 59.74 ± 3.29 |
| emQL-like                    | 23.06 ± 1.12 | 6.78 ± 2.24 | 19.86 ± 4.99 | 53.36 ± 3.46 | 81.73 ± 3.63 | 2.17 ± 0.57 | 48.54 ± 5.09 |
| MPQE-like                    | 16.53 ± 0.48 | 3.81 ± 0.38 | 12.70 ± 1.59 | 41.61 ± 1.49 | 60.67 ± 2.23 | 6.84 ± 0.58 | 28.76 ± 1.40 |
| MPQE-like + Reif             | **25.52 ± 0.36** | 3.24 ± 0.62 | 10.52 ± 2.09 | 41.36 ± 0.50 | 63.93 ± 1.36 | 5.59 ± 0.72 | 18.75 ± 1.55 |
| **Hits@3 (%)**               |            |            |            |            |            |            |            |
| StarE-like                   | 35.58 ± 0.82 | **46.41 ± 0.32** | 57.34 ± 0.58 | 67.98 ± 0.93 | 87.56 ± 0.74 | **56.89 ± 0.47** | 75.35 ± 1.02 |
| Q2B-like                     | 38.79 ± 0.92 | 43.75 ± 0.98 | 55.41 ± 1.21 | 67.02 ± 1.24 | 87.97 ± 1.23 | 46.99 ± 3.04 | 71.20 ± 2.45 |
| emQL-like                    | 36.14 ± 1.11 | 10.73 ± 3.23 | 30.47 ± 6.37 | 66.56 ± 3.18 | 89.91 ± 2.87 | 3.80 ± 1.05 | 55.96 ± 5.31 |
| MPQE-like                    | 30.82 ± 0.75 | 7.15 ± 0.65 | 21.48 ± 2.58 | 66.87 ± 1.21 | 86.17 ± 1.45 | 10.08 ± 1.08 | 44.88 ± 1.30 |
| MPQE-like + Reif             | **41.26 ± 0.65** | 6.34 ± 0.82 | 18.25 ± 2.69 | **68.14 ± 0.97** | 90.07 ± 0.58 | 8.56 ± 0.59 | 32.31 ± 2.60 |
| **Hits@10 (%)**              |            |            |            |            |            |            |            |
| StarE-like                   | 51.72 ± 0.66 | **51.20 ± 0.44** | 65.50 ± 0.39 | 77.78 ± 0.53 | 92.64 ± 0.65 | **61.81 ± 0.37** | 81.60 ± 0.60 |
| Q2B-like                     | 55.44 ± 1.35 | 51.10 ± 1.40 | **66.39 ± 1.72** | 78.79 ± 1.04 | 94.20 ± 0.86 | 57.49 ± 2.26 | 80.49 ± 1.92 |
| emQL-like                    | 50.10 ± 1.34 | 16.45 ± 3.56 | 44.36 ± 4.96 | 75.86 ± 2.45 | 93.55 ± 1.93 | 6.79 ± 1.13 | 62.80 ± 5.26 |
| MPQE-like                    | 48.48 ± 0.59 | 12.57 ± 0.96 | 34.19 ± 3.78 | 83.04 ± 1.01 | 96.32 ± 0.77 | 14.75 ± 1.42 | 61.02 ± 0.70 |
| MPQE-like + Reif             | **58.43 ± 0.29** | 12.02 ± 1.12 | 31.14 ± 2.70 | **83.77 ± 0.47** | 97.22 ± 0.14 | 13.50 ± 0.81 | 50.92 ± 3.44 |
| **MRR (%)**                  |            |            |            |            |            |            |            |
| StarE-like                   | 30.98 ± 0.91 | **44.13 ± 0.28** | 52.96 ± 0.61 | **63.14 ± 0.97** | 83.78 ± 1.00 | 55.20 ± 0.52 | **71.52 ± 1.37** |
| Q2B-like                     | 33.04 ± 0.84 | 41.99 ± 0.88 | 51.71 ± 1.18 | 61.72 ± 1.18 | 83.49 ± 1.24 | 44.24 ± 2.73 | 67.04 ± 2.70 |
| emQL-like                    | 32.01 ± 1.00 | 10.09 ± 2.70 | 27.94 ± 5.11 | 61.45 ± 3.13 | **86.28 ± 3.11** | 3.73 ± 0.94 | 53.58 ± 5.03 |
| MPQE-like                    | 26.83 ± 0.53 | 6.79 ± 0.56 | 19.72 ± 2.23 | 56.16 ± 1.30 | 74.35 ± 1.70 | 9.62 ± 0.85 | 39.81 ± 1.20 |
| MPQE-like + Reif             | **36.36 ± 0.38** | 6.12 ± 0.74 | 17.11 ± 2.27 | 56.81 ± 0.69 | 77.29 ± 0.86 | 8.32 ± 0.52 | 29.25 ± 2.05 |
| **AMRI (%)**                 |            |            |            |            |            |            |            |
| StarE-like                   | 78.44 ± 1.78 | 68.11 ± 2.52 | 74.62 ± 2.94 | 93.63 ± 0.81 | 98.65 ± 0.33 | 73.14 ± 2.39 | 88.76 ± 0.61 |
| Q2B-like                     | 88.69 ± 0.45 | **87.17 ± 1.48** | 95.60 ± 0.58 | 99.01 ± 0.20 | 99.93 ± 0.03 | 83.24 ± 1.08 | 98.49 ± 0.40 |
| emQL-like                    | 73.20 ± 11.74 | 51.74 ± 13.25 | 74.93 ± 10.70 | 90.68 ± 5.62 | 97.79 ± 1.60 | 37.80 ± 22.89 | 82.59 ± 8.45 |
| MPQE-like                    | 93.77 ± 0.99 | 83.25 ± 2.61 | 92.00 ± 3.04 | 99.49 ± 0.05 | 99.96 ± 0.01 | 85.61 ± 2.86 | 99.04 ± 0.16 |
| MPQE-like + Reif             | **95.68 ± 0.09** | 82.93 ± 1.83 | 92.08 ± 1.43 | **99.57 ± 0.02** | **99.97 ± 0.00** | **86.54 ± 1.56** | **99.25 ± 0.06** |