Top-k User-Defined Vertex Scoring Queries in Edge-Labeled Graph Databases

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We consider identifying highly ranked vertices in large graph databases such as social networks or the Semantic Web where there are edge labels. There are many applications where users express *scoring queries* against such databases that involve two elements: (i) a set of patterns describing relationships that a vertex of interest to the user must satisfy and (ii) a scoring mechanism in which the user may use properties of the vertex to assign a score to that vertex. We define the concept of a partial pattern map query (partial PM-query), which intuitively allows us to prune partial matchings, and show that finding an optimal partial PM-query is NP-hard. We then propose two algorithms, PScore_LP and PScore_NWST, to find the answer to a scoring (top- k) query. In PScore_LP, the optimal partial PM-query is found using a list-oriented pruning method. PScore_NWST leverages node-weighted Steiner trees to quickly compute slightly sub-optimal solutions. We conduct detailed experiments comparing our algorithms with (i) an algorithm (PScore_Base) that computes all answers to the query, evaluates them according to the scoring method, and chooses the top- k , and (ii) two Semantic Web query processing systems (Jena and GraphDB). Our algorithms show better performance than PScore_Base and the Semantic Web query processing systems—moreover, PScore_NWST outperforms PScore_LP on large queries and on queries with a tree structure.

CCS Concepts: • **Information systems** → **Data structures**; **Information retrieval query processing**; **Retrieval models and ranking**;

Additional Key Words and Phrases: Graph databases, scoring queries, top- k querying

ACM Reference format:

Francesco Parisi, Noseong Park, Andrea Pugliese, and V. S. Subrahmanian. 2018. Top-k User-Defined Vertex Scoring Queries in Edge-Labeled Graph Databases. *ACM Trans. Web* 12, 4, Article 21 (September 2018), 35 pages.

<https://doi.org/10.1145/3213891>

F. Parisi and N. Park equally contributed to the paper.

Some of the authors may have been partly funded by ONR Grants No. N000141612739, No. N000141512007, No. N000141612896, and No. N000141512742, by ARO Grant No. W911NF1410358, by the Start-(H)Open POR Grant No. J28C17000380006 funded by the Calabria Region Administration, and by the NextShop PON Grant No. F/050374/01-03/X32 funded by the Italian Ministry for Economic Development.

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<https://doi.org/10.1145/3213891>

1 INTRODUCTION

Edge-labeled graph databases are becoming increasingly important. Many online social networks can be viewed as edge-labeled graphs. For instance, in LinkedIn, users are vertices. An edge (u, v) from user u to user v may exist with a friend label if u friended v (and v accepted), a pfriend label if u friended v but was not accepted, and a host of labels endorsed- t if u endorsed v w.r.t. topic t and not_endorsed- t if u was given the option of endorsing v for topic t but did not do so. Likewise, LinkedIn may also consider companies and employers to be vertices, universities, and schools to be vertices, and place edges between persons and such vertices labeled with relationships like employs or alumnus_of with the obvious meaning. On Twitter, vertices might include user handles, locations (from profiles), and hashtags that either appear on people's profiles or tweets. A follows edge from u to v might indicate that u follows v , a location edge from u to a location indicates that u is from that location, and an interest edge from u to v might indicate that u is interested in hashtag v . Thus, edge-labeled graphs can play an important role in capturing many of the semantic relationships explicitly mentioned in many social networks. Likewise, the *(subject, property, object)* triples used in RDF can be viewed as edge-labeled graphs where there is an edge from a subject to an object vertex.

While there has been extensive work on top- k queries on ordinary graphs [11, 15, 42, 52], there has been no work on top- k queries on edge-labeled graphs where the user gets to choose what is considered important when she is articulating her query, i.e., the concept of importance is expressed in the user query—in contrast, in most past work, the system imposes an *a priori* definition of importance. This capability of expressing importance-scoring methods within the query provides huge flexibility and capability to the user, and tends to be hard to index because we do not know, *a priori*, what the user's query and scoring method will be.

1.1 Motivating Examples

Consider a simple nuclear proliferation example in which an analyst is trying to identify suspicious entities. The analyst already has a network consisting of vertices (people, companies) and links between them. For instance, SPINN [1] extracts this network by first finding individuals/companies who have been sanctioned by the US and other similar governments for export control violations. SPINN then uses LinkedIn and Bloomberg's worldwide lists of directors and officers of companies to flesh this network out completely. Of course, not everyone in the SPINN's network of over 74K vertices and over 1M edges is necessarily bad. The suspiciousness level is represented as one of $\{1, 0, -1\}$ —each represents “suspicious,” “unknown,” and “non-suspicious,” respectively.

Our knowledge of nuclear proliferation networks that have been previously discovered suggests some typical suspicious connections among suspect vertices. Two anonymized example pattern queries created from them are shown in Figure 1, one corresponding to a suspicious financial network, and another corresponding to a suspicious logistics network—both these can be illicit networks because money and materials must both be “moved” to achieve a desired goal. The query PQ_1 looking for suspicious financial networks starts by focusing on the suspicious bank $B1$ —which has come to the notice of nuclear regulators for a reason. They are looking for banks matched for $?b1$ (through a path of “partner” links of maximum length 2), which has financed an energy company $?c2$ and a metallurgy company $?c1$. Such a subnetwork might be suspicious because bank $?b1$ is financing nuclear supply producers. PQ_2 , similarly, is looking for logistics companies $?c1$ and $?c2$ that are partners of the suspicious logistics companies $C7$ and $C8$, as well as two people $?p1$, $?p2$, and a bank $?b1$. Bank $?b1$ must have funded both $?c1$ and $?c2$. $?p1$ and $?p2$ must have friendship and are both linked to the suspicious logistics companies. If the same bank appears as a solution to $?b1$ in both queries, then it would naturally be of greater interest to the analyst.

Fig. 1. Example query. Circles represent people, diamonds represent companies, and rectangles represent banks. An edge annotated with an integer number w can be matched to paths with maximum length w .

Fig. 2. Example graph database $\mathcal{G}$. Vertices are annotated with the values of their *suspicious* and *specialty* properties; integers represent suspiciousness levels; M stands for metallurgy, L stands for logistics, and E stands for energy.

To this end, we score matched patterns of each query with $?c1.sus + (1 + ?c2.sus)^2$ and project to $?b1$. In both queries, $?c2$ plays a more important role for nuclear proliferation. A vertex score in each query is then defined as an aggregated value (we use SUM in the example) over the scores of all patterns projected to the same vertex. Finally, we total the vertex score of each query up. With the simple SPINN network example of Figure 2, one pattern of PQ_1 maps $?b1$ to B2— $?b2$ is mapped to B4, $?c1$ to C2 and $?c2$ to C1, so B2's score is $1 + (1 + 1)^2 = 5$ for PQ_1 . Two patterns of PQ_2 map $?b1$ to B2. In the first one, $?c1$ is mapped to C6, $?c2$ to C1, $?p1$ to P4, and $?p2$ to P1, so B2's score is $0 + (1 + 1)^2 = 4$. In the second one, $?c1$ is mapped to C2, $?c2$ to C1, $?p1$ to P3, and $?p2$ to P1, so B2's score is $1 + (1 + 1)^2 = 5$. Thus, the overall score of B2 w.r.t. PQ_2 is 9, and its score is 14 if we use SUM to aggregate scores (the scores of B3, B4, and B6 are 6, 4, and 1, respectively).

Queries such as this require the following features: (i) The user must be able to specify a set of patterns of interest to her. (ii) The user must be able to specify a scoring function that extracts properties of a vertex ($?c1.sus$ above) and use it to define a scoring metric. (iii) The user must be

Fig. 3. Example query patterns for the medical insurance fraud scenario.

able to specify maximum path lengths in her query. (iv) The user must be able to “bump up” the score of a vertex that satisfies multiple criteria by aggregating them (as is done by adding up the two scores above).

The use of patterns similar to those in the SPINN nuclear trafficking application applies in many different commercial fraud investigations as well. For instance, one type of medical insurance fraud (MIF) involves staging fake accidents. The individuals and organizations involved in such MIF networks involve a network of individuals (called “runners”) who stage accidents and bring fake “victims” to one or more “clinics.” Another network of individuals handle the legal side of things—they involve networks of lawyers and claimants who work closely together in the scam. A third network of individuals include the medical professionals and doctors who deliver the medical services—doctors involved in the fraud are often connected with other doctors. And a fourth network ties the clinics involved that ultimately bill the insurance company. Often times, the same patient visits many different clinics, and the same doctors are tied to different clinics involved in the fraud, and so are the lawyers. A person who ends up occurring in many of these networks is generally more suspicious than others. Insurance investigators wish to specify methods to focus on the most suspicious individuals—something that can be expressed via the scoring queries (S-queries) proposed in this article—and they are generally looking for the top- k suspicious people as they are limited in their investigative resources.¹ Because the MIF pattern is so complex, there are a whole range of possible graph patterns that fraud investigators might look for. Figure 3 shows three such graph patterns. The first one wishes to find lawyers (?l1) and doctors (?d1, ?d2) who are involved in claims and are linked to the Smith law firm, which may be suspicious for various reasons. The second and third patterns are different patterns that are also looking for doctors and lawyers linked in a different way to a different law firm.

If the same lawyer and/or the same doctors show up many different times in the answers to one or more of these patterns, they have to be considered more suspicious. For instance, the same doctor or the same lawyer might be involved in many different claims. In such cases, we would like to assign a higher score to the ?l1, ?d1, ?d2 variables. One way an investigator might do this is by defining the score of such variables as $\frac{?c.claim_amount}{10K} + ?x.work_years$, where $?x \in \{?l1, ?d1, ?d2\}$ —this scoring function also considers a person’s skills in her area of work.

And of course, if the same doctor/lawyer shows up as an answer across more than one of these three patterns, she has to be considered even more suspicious. Hence, the investigator could define the final score of the doctor or lawyer as the sum of their scores across the different patterns.

In general, the fraud investigator has limited resources to carry out physical and/or electronic surveillance of these suspicious entities. She wishes to assign a suspicion score to doctors/lawyers so she can focus her limited resources on those most likely involved in the fraud. This is why

¹See <http://linkanalysisnow.com/2009/04/analyzing-medical-fraud.html> for a detailed analysis of how such scams work. This site also provides links to lots of other fraudulent activities where scoring queries may play a natural role.

she uses the scoring functions shown above to capture her suspicion of the different doctors and lawyers known to the insurance company.

The above two examples, one each on identifying suspicious vertices in nuclear proliferation investigations, as well as in identifying suspicious vertices in MIF, are special cases of broader investigations into different types of illicit activity. The same principles apply to other types of complex crime networks such as money laundering networks, drug networks, human trafficking networks, to name a few. Investigations to identify suspicious vertices in all of these networks are critical because there are limited resources for carrying out physical and/electronic surveillance. In some cases, they are downright dangerous (e.g., to place an undercover officer in the illicit network). This is why the complexity of the query language is not important from an application perspective—rather, the query language must allow the investigator to articulate precisely the patterns of interest to her, together with her own methods for scoring. Simply put, lives may depend on it, at least in such applications.

As it will be discussed in detail in Section 2, many of the query models proposed in the past do not perform aggregation but rather concentrate on individual patterns—our model is conceptually more similar to SQL queries with both GROUP BY and ORDER BY clauses. The different existing models obviously have different possible applications—however, costly algorithms are usually needed to process GROUP BY queries. One key aspect of our proposed model is also its capability to handle graph queries equipped with very flexible scoring functions, so that users are able to conduct more sophisticated pattern-matching tasks such as the ones described above.

1.2 Plan of the Article

The rest of the article is organized as follows. Section 2 describes related work. Then, in Sections 3 and 4, we define graph databases, propose *S-queries* that capture the above features, and define the top-*k* answers to *S-queries*. Section 5 describes our *S-query* processing algorithm. The algorithm includes a method to estimate an upper bound on the score of any vertex that allows us to prune the search for top-*k* answers. The estimation of these upper bounds is critical, but unfortunately, exactly finding these upper bounds is NP-hard. Because of this, we present two algorithms: the PScore_LP algorithm where the optimal upper bound is found using a list-oriented pruning method, and the PScore_NWST algorithm, which leverages node-weighted Steiner trees (NWSTs) to quickly find very good upper bounds (though they may not be optimal). Section 6 discusses how our approaches can be extended to encompass any maximum path length constraints expressed in the query. Section 7 summarizes our experiments on seven real-world datasets involving graphs with up to 234M edges.

2 RELATED WORK

Subgraph matching has been extensively studied [11, 18, 31, 35, 42, 49, 54]—surveys of the work in this field can be found, e.g., in References [27], [29], [22].

Some approaches (e.g., References [11, 42]) map edges in the query to paths in the graph—these approaches may constrain path lengths but do not try to identify top-*k* vertices. Instead, they focus on finding patterns in the graph data that are isomorphic to a given query pattern—the isomorphisms yield substitutions that assign vertices in the graph to variables in the expressed patterns. We leverage some of these works in this article in terms of the edge to path mappings, as we allow single query edges to be mapped to paths in the graph. Others try to find the top-*k* substitutions in different situations. The HRJoins proposed in Reference [42] are targeted at twig queries on graph data, in which substitutions are scored (not vertices as we do). The score of a substitution is the sum of the edge weights of all edges involved in the edge to path mappings. The concept of kGPM queries is used in Reference [11] to extend this work to graph data. They score answer

substitutions using the sum of edge weights. The k most similar subgraphs to a query graph, where similarity is defined using maximum common subgraphs, are targeted in Reference [54] with the introduction of the DPIndex, OPIIndex, and GSIndex structures.

In the LONA framework proposed in Reference [52] for top- k queries, the user does not specify patterns, but vertices in the graph are scored via a function f . This is a relevance score for each vertex. Once these relevance scores are computed, the authors compute a higher-level score that aggregates the lower-level relevance scores of a vertex and all its neighbors within some number of hops specified in the query. The aggregation is computed as $\sum_{u \in Nbr(v, h)} f(u)$, where $Nbr(v, h)$ is a set of h -hop neighbors of v . Top- k vertex set search by graph simulation has been suggested in Reference [15], where the score of the output variable of a single-pattern query is defined as the size of the maximum graph simulation matching the output variable to a vertex. Both the above approaches do not allow the user to specify multiple patterns in the query nor to choose the scoring function.

The concept of graph database used in this article is similar to that of the Heterogeneous Information Network (HIN) [48], which is modeled as a directed graph where vertices and edges are annotated with types. In a graph database, each vertex is associated with multiple properties, including type, and edges are associated with labels that can be viewed as types. Thus, graph databases generalize HINs by allowing multiple properties to be associated with vertices. A relevant problem investigated in HINs is measuring similarity between vertices [44]. In this regard, using the “meta-paths” semantics (i.e., paths defined on the schema-level graph of the vertices’ types), Reference [48] proposed *PathSim*, a meta-path-based similarity measure for evaluating the similarity of same-typed vertices based on symmetric paths. Meta-paths are a special case of meta-structures [24] that consist of a direct acyclic (schema-level) graph with a single source vertex and a single target vertex. In Reference [24], to measure the relevance of two vertices, measures are proposed that are based on looking at the number of sub-graphs that match a meta-structure—this is done through sub-graph expansion restricted to a meta-structure. Symmetric metagraphs similar to meta-structures are exploited in Reference [16], where a supervised approach to proximity search is proposed. They aim at learning weights for optimally aggregating different characteristic metagraphs that specify classes of semantically similar objects. This can be viewed as aggregating multiple query patterns, but the end-user does not take part in the process, which is designed to automatically learn weights for combining different metagraphs. Different from the above-mentioned approaches, we do not rank vertexes by measuring their proximity to a query vertex in terms of the (weighted) numbers of meta-paths instances, but compute top- k answers on the basis of user-defined (local and global) aggregation functions that are evaluated on vertices once the patterns provided in the query are fully mapped to the graph data.

The MAGE system proposed in Reference [41] supports exact and approximate subgraph matching on graphs with both vertex and edge attributes, for which wildcards and multiple values attributes are allowed. The k desired matching subgraphs are ranked through a (fixed) proximity measure based on multiplying the RWR (Random Walk with Restart) values of the pairs of vertices in the graph that instantiate pairs of vertices in the query. Finally, the graph-querying framework NeMa proposed in Reference [28] allows for ambiguity in both the structure and vertex labels. Instead of checking graph isomorphism, NeMa identifies top- k optimal matches by minimizing vertex labels differences (using Jaccard similarity measure) and vertex pairs distances. Thus, it is designed to possibly return results that deviate from the given query pattern.

It is also worth noting the importance of handling multiple query patterns “by design.” In fact, the user brings her own preferences and knowledge during the whole process of query definition—from the definition of the local scores for the query patterns she believes are more significant, to the choice of a global function for aggregating single patterns’ scores. This is a simple, yet crucial

difference with some of the approaches discussed above. Indeed, though, in principle, existing techniques could handle multiple query patterns by processing single query patterns one by one and then aggregating the scores in a custom way, there are several issues that can make it relatively impractical for the user to understand the meaning the final answer obtained. In fact, most of the other approaches define the (local) scores of top- k answers of single query patterns by ranking the obtained substitutions through predefined functions that the user is supposed to use as a black box (for instance, RWR multiplication in MAGE). Moreover, it is in general not easy to determine the k' value the user should use to extract top- k' intermediate answers to single patterns and then build the final top- k answers over multiple patterns. To obtain this, existing techniques may need to apply “exhaustive” approaches based on the maximum possible value of k' for the intermediate answers. To see why, consider for instance a simple case where the (local) scores obtained using two single query patterns are $s_1 = \{5, 3, 2\}$ and $s_2 = \{3, 2, 1\}$, respectively, and we are interested in extracting the top-1 answer obtained by averaging local scores. In this case, taking the average of any top- k' subset of s_1 or s_2 , for any $k' < 3$, would result in a wrong top-1 final score.

As a final remark, we point out that relevant work has focused on the storage and querying of RDF data [2–5, 8, 10, 14, 19, 20, 26, 38, 40, 43, 51, 56] and its associated SPARQL query language [23]. Our proposed vertex importance queries can be expressed in SPARQL through the use of GROUP BY, UNION, LIMIT, and ORDER BY operators, and by “expanding” queries into equivalent sets of queries without edge length constraints (SPARQL “property paths” do not allow such constraints). However, the majority of the approaches to RDF storage and querying are based on traditional relational storage techniques that are known to have lower performance than graph databases when answering subgraph matching queries, due to the large number of joins needed on the tables representing the structure of the graph [2, 10, 43]. In particular, the approaches used in many existing RDF query engines (e.g., References [8, 26, 47, 51]) severely limit the actual usability of property paths, due to the huge computational effort needed to join the tables built [2]. Neo4j [36], Titan [50], and DOGMA [7] (Titan’s original research work) provide (recursive) graph-traversal subgraph-matching algorithms based on proprietary graph indexing schemes (to avoid table joins). We employ the DOGMA algorithm as a basis for our mapping algorithm. Specific top- k query processing algorithms for RDF or social network data have been proposed as well (e.g., References [32], [39], [53], and [55]). However, they are mainly interested in scoring substitutions (or projections of substitutions) without aggregation. In particular, the ranked matching (RM) algorithm [55] scores substitutions of a query pattern by summing up, for each vertex v of a query, the pairwise similarity between v and its matching in the graph. A function providing the similarity values, for each pair of vertices in the graph, is assumed as input of the algorithm, and simple data graphs without labels are considered. Attributed graphs are instead considered in Reference [39], where OptIQ (Optimized Importance Query) algorithm is introduced for computing top- k answers that are obtained by ranking substitutions with user-defined scoring functions without aggregation. The STAR framework [53] reduces the computation of top- k answers to a (general) graph query to the computation of the answers to a set of star-shaped queries. The top- k answers to each star query are defined by ranking substitutions, each of them scored by summing up the similarity scores of the vertices and edges that match the query pattern. Specifically, weighted aggregation of different similarity functions (provided by the system, not by the end-users) can be used to define the score of each vertex, and matching a single edge to a path of bounded length is allowed. In general, the above approaches score substitutions (or projections of substitutions) without aggregation—thus, they only focus on ORDER BY and LIMIT queries that suffice for their purpose.

The features of some of the above related works are summarized in Table 1, where, in the “top- k ” column, symbol V (resp. S) means that that work addresses the problem of identifying the top- k vertices (resp. substitutions).

Table 1. Comparison with Related Work

	Multiple patterns	Vert. prop.-based scoring	Path edges	Global scoring	Top- k
kGPM [11]	–	–	✓	–	✓ (S)
HRJoins [42]	–	–	✓	–	✓ (S)
Simulation [15]	–	–	✓	–	✓ (V)
LONA [52]	–	✓	–	–	✓ (V)
DPInd., OPInd., GSInd. [54]	–	–	–	–	✓ (S)
PathSim [48]	–	–	–	–	✓ (S)
Meta Structure [24]	–	–	–	–	✓ (S)
Meta Graph [16]	✓	–	–	✓	✓ (S)
MAGE [41]	–	–	–	–	✓ (S)
NeMa [28]	–	–	–	–	✓ (S)
STAR [53]	–	–	✓	–	✓ (S)
RM [55]	–	–	–	–	✓ (S)
OptIQ [39]	–	✓	–	–	✓ (S)
This work	✓	✓	✓	✓	✓ (V)

3 GRAPH DATABASES

We assume the existence of four arbitrary, but fixed, disjoint sets $V, \mathcal{L}, \mathcal{P}, \mathcal{T}$ of *vertex names*, *edge labels*, *vertex properties*, and *type names*, respectively. Each $p \in \mathcal{P}$ has an associated domain $dom(p)$, which is a set (disjoint from $V, \mathcal{L}$, and $\mathcal{P}$) of values that can be assigned to p . We assume the existence of a special property *type* $\in \mathcal{P}$ with domain $\mathcal{T}$. A graph database is defined as follows.

Definition 3.1 (Graph Database). A Graph Database $\mathcal{G}$ is a triple $\langle V, E, \wp \rangle$, where

- $E \subseteq V \times \mathcal{L} \times V$ is a set of labeled edges;
- $\wp : V \times \mathcal{P} \rightarrow \bigcup_{p \in \mathcal{P}} dom(p)$ is a (possibly partial) *property assignment* function, such that
 - (i) if $\wp(v, p)$ is defined, then $\wp(v, p) \in dom(p)$, and (ii) $\wp(v, type)$ is defined for all $v \in V$.²

In our running example, the set of types may include person, company, bank, and more. A sample graph database is shown in Figure 2. If $\mathcal{P} = \{type, suspicious, specialty\}$ and $dom(type) = \{person, company, bank\}$, the property function assigns the value *person* to the pair $(P1, type)$, meaning that *person* is the type of the vertex named *P1*.

In the remainder of the article, we assume an arbitrary but fixed graph database $\mathcal{G} = \langle V, E, \wp \rangle$ is given.

4 SCORING QUERIES

In this section, we formally define S-queries, an example of which was informally given in the Introduction. An S-query consists of a set of *Pattern Map Queries* (PM-queries) as shown by the graphs in Figure 1 and a global aggregation function, according to which the scores of answers generated by the individual PM-queries can be evaluated. Intuitively, a PM-query is used to specify a way to (locally) score a class of sub-graphs of $\mathcal{G}$ having some characteristic (structure, vertex properties,

²We assume that every vertex has a *type* property because vertices have types (or types can be inferred) in the majority of real world scenarios, and this is a valuable additional information used by our index structure (see Section 5.2). In the absence of types, we can simply assign a unique fictitious type to all vertices in the database and queries.

Table 2. Symbols Used

Symbol	Section	Meaning
$\wp$	3 (Definition 3.1)	Property assignment function
$\mathcal{G} = \langle V, E, \wp \rangle$	3 (Definition 3.1)	Graph database
χ	4.1 (Definition 4.1)	Set of constraints over variables
ϱ	4.1 (Definition 4.1)	Function that associates variables with numerical terms
la	4.1 (Definition 4.1)	Local aggregation function
$PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$	4.1 (Definition 4.1)	PM-query
ga	4.1 (Definition 4.2)	Global aggregation function
$SQ = \langle PQS, ga \rangle$	4.1 (Definition 4.2)	S-query (PQS is a set of PM-queries)
$lscore(v, PQ)$	4.1 (Definition 4.4)	Local score of v w.r.t. PQ
$score(v, SQ)$	4.1 (Definition 4.5)	Score of v w.r.t. SQ
$ans(SQ)$	4.1 (Definition 4.6)	Top- k answer to SQ
$\mathcal{E}(PQ)$	5.1	Set of essential variables in PQ
PPQ	5.1 (Definition 5.1)	Partial PM-query for PQ
$score^*(v)$	5.2	Upper bound on $score(v, SQ)$
$sub^*(PQ)$	5.2	Upper bound on the number of answer substitutions for PQ
$cand(v, \delta, \pi, (l, d))$	5.2	Number of vertices that are connected to v via an undirected path of length δ ending with an edge labeled ℓ of type π with direction d
$cand^*(PQ, ?x)$	5.2	Upper bound on the number of substitutions for variable $?x$ in PQ
$opt(PQ)$	5.3	Chosen partial PM-query for PQ
$sub^*(PPQ, PQ)$	5.3	Upper bound on the number of substitutions for the variables in PQ that are not in PPQ
PScore	5.4	General query processing algorithm
PScore_LP	5.4	PScore algorithm with list-oriented pruning
PScore_NWST	5.4	PScore algorithm with NWST-based pruning
$eq(PQ)$	6.1	Equivalent set of non-annotated “expanded” PM-queries for PQ
$cov(PPQ)$	6.1	Subset of $eq(PQ)$ such that, by extending a substitution for PPQ , full substitutions for all the queries in the subset can be obtained

or edge labels) the user wants to look for. Table 2 summarizes the symbols used throughout the article.

4.1 Pattern Map Queries

Let VAR be a set of variable symbols (we use strings starting with question marks as for variables). We assume VAR is disjoint from $V, \mathcal{L}, \mathcal{P}, \mathcal{T}$ and from $\bigcup_{p \in \mathcal{P}} dom(p)$. The idea is that variables must be “bound” to vertices in the graph database. A (*numerical*) *term* is a value of a property, a property of a query variable, a real number, or a polynomial-time computable function of terms. For instance, $(?x.sus - 1)$, $(?x.sus + 1) * (?y.sus + 2)$ are all terms. A *constraint* is a comparison between terms, the application of a set operator to terms, or the application of a logical operator ($\wedge$, $\vee$, or $\neg$) to

constraints. For instance, $Energy \in ?x.specialty$, $?x.sus > ?y.sus$, and $(?x.sus > 0 \wedge ?x.sus \leq y.sus + 1)$ are all constraints.

We are now ready to introduce the notion of pattern map query (PM-query). Let $*$ be a distinguished “wildcard” label not occurring in $\mathcal{L}$.

Definition 4.1 (Pattern Map (PM) Query). A PM-query is a 5-tuple $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$, where:

- $V_{PQ} \subseteq V \cup VAR$ with $V_{PQ} \cap V \neq \emptyset$.
- $E_{PQ} \subseteq V_{PQ} \times (2^{\mathcal{L}} \cup \{*\}) \times \mathbb{Z}^+ \times V_{PQ}$.
- χ is a finite set of constraints over variables in V_{PQ} .
- ϱ is a partial function that associates variables in V_{PQ} with numerical terms.
- $la \in \{MIN, MAX, AVG, SUM\}$ is a “local” aggregation function.

We assume that every variable in V_{PQ} has a type constraint. In addition, if $\varrho(?x)$ is defined and its value is t , then we say that $?x$ is an *output variable*, t is a *scoring term*, and any variable occurring in t is a *scoring variable*. Moreover, if E_{PQ} contains an edge $e = (v, L, w, v')$ with $w > 1$, then we say that e is *annotated* and PQ is *edge-annotated*.

The first two items of Definition 4.1 say that a PM-query is a directed edge-labeled graph where (i) each vertex is either a vertex name or a variable symbol and (ii) each edge is labeled with a pair consisting of a set of edge labels (or $*$) and an integer. Intuitively, the user uses this graph to specify the structure of the sub-graphs of $\mathcal{G}$ she is looking for (where $*$ matches any label), including constraints about the maximum length of paths. The constraints in χ express requirements about vertex properties. Function ϱ provides a flexible way for ranking the vertices the user is interested in by means of (possibly complex) scoring terms, while la is a local aggregation function that tells us how scoring terms are aggregated. Finally, output variables are those that will be mapped to the vertices the user wants to compute local scores for, whereas scoring variables are those that will be mapped to the vertices that contribute to such scores.

It should be observed that we only consider *anchored* queries, that involve at least one constant. Anchored queries are considered of fundamental importance in many scenarios—for instance, anchors are present in (i) all queries in both the *DBPedia* [34] and *LUBM* [30] SPARQL benchmarks, (ii) 14 out of 20 queries in the *interactive* use case of the *Social Network Intelligence BenchMark* [45], (iii) 19 out of 20 queries in the *explore* and *business intelligence* use cases of the *Berlin* benchmark [6], and (iv) 14 out of 15 queries in the *SP²Bench* benchmark [46].

An S-query consists of a set of PM-queries along with a global aggregation function that combines the scores returned by each PM-query.

Definition 4.2 (Scoring Query). An S-query is a pair $SQ = \langle PQS, ga \rangle$, where PQS is a finite set of PM-queries and $ga \in \{MIN, MAX, AVG, SUM\}$ is a “global” aggregation function.

For instance, if we consider the PM-queries PQ_1 and PQ_2 of our running example, $SQ = \langle \{PQ_1, PQ_2\}, SUM \rangle$ is an S-query that ranks banks by the sum of the scores obtained from PQ_1 and PQ_2 .

To define the *answer* to a PM-query and an S-query, we need some intermediate concepts.

A *substitution* θ is a mapping $\theta : VAR \rightarrow V$. Applying θ to an expression e (vertex, term, or constraint) means replacing every variable $?x$ in e with vertex name $\theta(?x)$, and the ground (i.e., variable-free) expression resulting from such an application is denoted $e\theta$. Ground terms and ground constraints are evaluated in the obvious way.

Definition 4.3 (Answer Subst. for a PM-query). Given a PM-query $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$, an *answer substitution* θ for PQ is a mapping $\theta : V_{PQ} \rightarrow V$ such that

- for each $(\alpha, L, m, \beta) \in E_{PQ}$, there is path $(v_1, \ell_1, v_2), (v_2, \ell_2, v_3), \dots, (v_{m'}, \ell_{m'}, v_{m'+1})$ in $\mathcal{G}$ with $m' \leq m$ such that $v_1 = \alpha\theta$, $v_{m'+1} = \beta\theta$, and, for each $i \in [1..m']$, $\ell_i \in L$ if $L \neq \{*\}$;
- for each constraint $C \in \chi$, $C\theta$ evaluates to true.

For instance, two answer substitutions for PQ_1 of our running example are $\{?b1/B3, ?c1/C4, ?c2/C3, ?b2/B5\}$ and $\{?b1/B6, ?c1/C5, ?c2/C6, ?b2/B7\}$.³

The existence of an answer substitution θ for a PM-query PQ guarantees that there is a way of mapping all the variables in PQ to vertices of $\mathcal{G}$ so that it satisfies all other requirements specified by PQ : presence of vertex names specified in the query, paths having a given maximum length with appropriate edge labels, and vertex properties satisfying the constraints.

Given an answer substitution θ for PQ , and an output variable $?x$ of PQ , the score of a vertex $v = ?x\theta$ in $\mathcal{G}$ can be computed by evaluating $\varrho(?x)\theta$, which results in a numerical value (obtained when the numeric term $\varrho(?x)$ is instantiated by θ). Thus, if a vertex $v \in \mathcal{G}$ is the result of applying an answer substitution θ to a variable $?x \in V_{PQ}$, then it has a (local) score obtained by using la to aggregate all the values $\varrho(?x)\theta$. This is captured formally below.

Definition 4.4 (Local Score). Let v be a vertex in $\mathcal{G}$, and $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$ a PM-query. Let S be the set $\{\varrho(?x)\theta \mid \theta \text{ is an answer substitution for } PQ \text{ and } v = ?x\theta\}$. The *local score of v w.r.t. PQ* , denoted $lscore(v, PQ)$, is $la(S)$ if $S \neq \emptyset$, and undefined otherwise.

For instance, in our running example, $lscore(B2, PQ_1) = 5$ and $lscore(B2, PQ_2) = 9$.

Given an S-query $SQ = \langle PQS, ga \rangle$ and a vertex v of $\mathcal{G}$, we compute a single score for v w.r.t. SQ by aggregating (via the global aggregate function) the local scores of v w.r.t. each PM-query $PQ \in PQS$.

Definition 4.5 (Score). Let v a vertex in $\mathcal{G}$ and $SQ = \langle PQS, ga \rangle$ an S-query. Let S be the set $\{lscore(v, PQ) \mid PQ \in PQS\}$. The *score of v w.r.t. SQ* is defined as $score(v, SQ) = ga(S)$ if $S \neq \emptyset$, and undefined otherwise.

In our running example, $score(B2, SQ) = 14$, $score(B3, SQ) = 6$, and $score(B4, SQ) = 4$.

The top- k answer to an S-query SQ is given by the set of vertices of $\mathcal{G}$ having the k highest scores.

Definition 4.6 (Top- k Answer to an S-query). Let $SQ = \langle PQS, ga \rangle$ be an S-query and $k \leq |V|$ a positive integer. The *top- k answer to SQ* is the set $ans(SQ) = \{v_1, \dots, v_k\} \subseteq V$ such that (i) for each $i \in [1..k-1]$, $score(v_i, SQ) \geq score(v_{i+1}, SQ)$; (ii) there is no vertex $v \in V \setminus ans(SQ)$ such that $score(v, SQ) > score(v_k, SQ)$.

In our running example, the top-2 answer to SQ is the set $\{B2, B3\}$.

5 QUERY PROCESSING

To efficiently compute the top- k answer to an S-query $SQ = \langle PQS, ga \rangle$, we perform the following steps:

- (1) We *partially match* the PM-queries in PQS .
- (2) We estimate *upper bounds* on the scores obtainable by vertices in $\mathcal{G}$.
- (3) We then progressively *extend* these partial matches. In the process, vertices that are no longer candidates to be in the top- k answer (since their upper bounds are lower than the current top- k) are pruned.

³We use *multisets* of substitutions in general, since two same substitutions with different intermediate edges between vertices, when edges are annotated, are counted twice [23].

Table 3. Essential Partial Substitutions for PQ_1 and PQ_2
(without Annotations). $\theta_{i,j}$ is the j -th Partial
Substitution for PQ_i

Substitution	?b1	?c1 (?c1.sus)	?c2 (?c2.sus)
$\theta_{1,1}$	B3	C4 (1)	C3 (0)
$\theta_{1,2}$	B3	C2 (1)	C3 (0)
$\theta_{1,3}$	B2	C2 (1)	C1 (1)
$\theta_{1,4}$	B2	C2 (1)	C6 (0)
$\theta_{2,1}$	B2	C6 (0)	C1 (1)
$\theta_{2,2}$	B2	C2 (1)	C1 (1)
$\theta_{2,3}$	B4	C2 (1)	C1 (1)
$\theta_{2,4}$	B3	C3 (0)	C2 (1)
$\theta_{2,5}$	B2	C3 (0)	C2 (1)

In this section, we describe the techniques we developed to support the above process in the case of non-annotated queries. Later, in Section 6, we discuss the extensions for the case of edge-annotated queries.

5.1 Partial Matching

In our approach, partial matching is performed by computing substitutions for a *subset* of the variables in a given PM-query PQ . A query variable is said to be *essential* if it is either an output variable or a scoring variable in PQ . We use $\mathcal{E}(PQ)$ to denote the set of all essential variables in PQ . For instance, in both the PM-queries of our running example, ?b1, ?c1, and ?c2 are essential variables. Formally, a partial matching is the application of a substitution to a *partial PM-query* extracted from PQ that includes a subset of vertices of PQ (containing all essential variables) and a subset of edges of PQ , as defined below.

Definition 5.1 (Partial PM-query). Given a PM-query $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$, a *partial PM-query* PPQ for PQ is a 5-tuple $PPQ = \langle V_{PPQ}, E_{PPQ}, \chi, \varrho, la \rangle$ such that:

- $\mathcal{E}(PQ) \subseteq V_{PPQ} \subseteq V_{PQ}$;
- $V_{PPQ} \cap V \neq \emptyset$;
- $E_{PPQ} \subseteq E_{PQ}$ is such that there exists at least one undirected path between every pair of essential variables in $\mathcal{E}(PQ)$, and at least one undirected path between each essential variable in $\mathcal{E}(PQ)$ and a constant vertex in V_{PPQ} .⁴

As an example, $?c1 \leftarrow ?b1 \ \& \ ?c2 \leftarrow ?b1 \leftarrow B1$ is a partial PM-query for PQ_1 of our running example (we sometimes abuse notation and use this shorthand notation for brevity).

Definition 5.2 (Essential Partial Substitution). Given a PM-query PQ , an *essential partial substitution* θ for PQ is an answer substitution for a partial PM-query of PQ .

Example 5.3. Consider the PM-queries of our running example, ignoring edge annotations for now. Observe that $?c1 \leftarrow ?b1 \ \& \ ?c2 \leftarrow ?b1 \leftarrow B1$ is a partial PM-query for PQ_1 , and $?c1 \leftarrow ?b1 \rightarrow ?c2 \ \& \ C8 \rightarrow ?c1 \leftarrow ?c2 \leftarrow C7$ is a partial PM-query for PQ_2 . The essential partial substitutions obtained in this case for PQ_1 and PQ_2 are reported in Table 3. Now, each vertex onto which a substitution maps variable ?b1 has a chance to be in the top- k answer. This chance may depend on the number of

⁴It should be observed that these paths *may* include a *subset* of the non-essential variables in PQ .

Table 4. Candidate Output Table for PQ_1 and PQ_2 (without Annotations)

Candidate output	Substitutions	Scoring term values
B2	$\theta_{1,3}, \theta_{1,4}, \theta_{2,1}, \theta_{2,2}, \theta_{2,5}$	5, 2, 4, 5, 4
B3	$\theta_{1,1}, \theta_{1,2}, \theta_{2,4}$	2, 2, 4
B4	$\theta_{2,3}$	4

full substitutions for the whole PM-queries PQ_1 and PQ_2 to which an essential partial substitution can be extended after mapping variables that do not belong to the partial PM-queries.

5.2 Computing Upper Bounds on Scores

Let us assume for now that, given an S-query $SQ = \langle PQS, ga \rangle$, we have chosen a partial PM-query for each $PQ_i \in PQS$ and we also have at hand all the possible essential partial substitutions for each of the partial PM-queries chosen.

We use these essential partial substitutions to compute upper bounds on local and global scores by creating a *candidate output table*, where for each candidate output vertex v , we maintain a list of essential partial substitutions that map an output variable to v , along with the values of the scoring terms obtained from the application of such substitutions. For instance, in the case of our running example, we create the candidate output table reported in Table 4.

Now, given a PM-query $PQ_i \in PQS$ with $la \in \{MIN, MAX, AVG\}$, we observe that an upper bound on $lscore(v, PQ_i)$ is the maximum among the scoring term values of v provided by all essential partial substitutions for PQ_i that map an output variable to v .

If $la = SUM$, it does not suffice to just include the scoring term value associated with a vertex v by an essential partial substitution θ for PQ_i in the computation of an upper bound on $lscore(v, PQ_i)$. Assume θ is computed for a partial PM-query PPQ_i of PQ_i . The scoring term value provided by θ must be multiplied by *an upper bound on the number of substitutions θ can be extended to after mapping the variables in PQ_i that were not chosen as variables of PPQ_i* . We compute this upper bound as $sub^*(PQ_i, \theta)$, where sub^* is a function that, given any PM-query PQ ,⁵ returns an upper bound on the number of answer substitutions for the query.

It should be observed that, although conceptually AVG is merely equal to SUM over the number of matches, in the case of AVG we still just take the maximum of the scoring term values as we do for MIN and MAX . The following example explains why this is necessary.

Example 5.4. Consider the case where we have computed a set $\{\theta_1, \dots, \theta_n\}$ of essential partial substitutions and their associated scoring term values are $x_1, \dots, x_n$ with $x_i \leq x_n$ for any $i \in [1..n]$. In this case, the correct upper bound under AVG is the maximum value x_n , because we must take into account the “extreme” case where θ_n is the only partial substitution that will eventually be extended to a full one. Including any $x_i < x_n$ in the computation would provide a lower value, thus an incorrect upper bound.

The above example also provides an intuition about why the proposed framework could be seamlessly extended to handle, e.g., $MODE$ and $MEDIAN$ (they can be treated the same way as MIN , MAX , and AVG) and $COUNT$ (which can be reduced to SUM by fixing scores to 1). In general, the framework immediately supports any aggregation function F such that, given a set X of values, it always holds that $MIN(X) \leq F(X) \leq MAX(X)$ (we call this family of functions “range-closed” in the remainder).

⁵Observe that $PQ_i\theta$ is a PM-query itself.

Table 5. Example Values of Function $cand$,
Where $\xleftarrow{\ell}$ Stands for (ℓ, in) and $\xrightarrow{\ell}$
for (ℓ, out)

v	δ	π	e	$cand$
B1	1	<i>bank</i>	$\xrightarrow{partner}$	2
B1	2	<i>company</i>	$\xrightarrow{funded}$	3
C2	1	<i>company</i>	$\xleftarrow{partner}$	3
C2	2	<i>bank</i>	$\xleftarrow{partner}$	1

Finally, an upper bound on $score(v, SQ)$, denoted $score^*(v)$, is obtained by applying the same reasoning to the aggregation of the local scores of v through function ga —the latter must therefore be range-closed as well.

Computing Upper Bounds on Substitutions. To quickly compute $sub^*(PQ)$, we employ a structure called *PM_Index*. This index provides a value $cand(v, \delta, \pi, e)$ for each vertex $v \in \mathcal{G}$, distance δ , value $\pi \in dom(type)$, and pair $e = (\ell, d)$, where $\ell \in \mathcal{L}$ and $d \in \{in, out\}$. This value is computed as follows:

- $cand(v, 1, \pi, e)$ is the cardinality of the set of vertices v' such that (i) $v'.type = \pi$ and (ii) $\mathcal{G}$ contains an edge (v, l, v') if $d = out$, an edge (v', l, v) otherwise.
- $cand(v, \delta, \pi, e) = \max\{cand(u, 1, \pi, e) \mid \text{there is an undirected path of length } \delta - 1 \text{ from } v \text{ to } u \text{ in } \mathcal{G}\}.$

Intuitively, for a given $(v, 1, \pi, e)$ quadruple (i.e., distance 1), the index contains, for each label ℓ , the number of in- and out-neighbors of v that are connected via an edge labeled ℓ that are of type π . The second part of the definition updates this for the case when $\delta > 1$ by recursively building on top of smaller values of δ .⁶ Some values of function $cand$ for the graph database of our running example are shown in Table 5.

Now, for each variable $?x$ in PQ , we can define an upper bound on the number of substitutions for $?x$ as $cand^*(PQ, ?x) = cand(v, \delta, \pi, e)$, where v is a constant vertex of PQ whose distance δ from $?x$ is minimum w.r.t. the other constant vertices of PQ , π is the value of the *type* property of $?x$, and the last edge of a shortest path between v and $?x$ is $(\cdot, \ell, ?x)$ if $e = (\ell, out)$, and $(?x, \ell, \cdot)$ otherwise.⁷

Finally, we can compute $sub^*(PQ)$ by multiplying the values of $cand^*(PQ, ?x)$ for all variables $?x$ in PQ . The following theorem ensures the correctness of this computation. The proofs for all the theorems in this article can be found in the Appendix.

THEOREM 5.5. *Suppose $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$ is a PM-query. Then,*

$$sub^*(PQ) = \prod_{?x \in V_{PQ} \cap VAR} cand^*(PQ, ?x)$$

is an upper bound on the number of substitutions for PQ .

⁶In the worst case, the construction of the *PM_Index* takes $O(|V|^2)$ time and its size is $O(|V|)$. However, our experiments on real datasets will show that actual construction times and index sizes are satisfactory in practice.

⁷We chose to use the shortest path in the definition of $cand^*(PQ, ?x)$ for simplicity. We could have used any other kind of path in the definition—Theorem 5.5 can easily be extended to hold anyway.

Example 5.6. In our running example, we have $sub^*(PQ_2) = \prod_{?V \in \{?b1, ?c1, ?c2, ?p1, ?p2\}} cand^*(PQ_2, ?V) = 12$ because $cand^*(PQ_2, ?c1) = cand(C8, 1, company, \xrightarrow{partner}) = 3$, $cand^*(PQ_2, ?c2) = cand(C7, 1, company, \xrightarrow{partner}) = 2$, and $cand^*(PQ_2, ?b1) = cand(C7, 2, bank, \xleftarrow{funded}) = 2$, $cand^*(PQ_2, ?p1) = cand(C8, 2, person, \xleftarrow{work}) = 1$, $cand^*(PQ_2, ?p2) = cand(C7, 2, person, \xleftarrow{work}) = 1$. Note that $C7$ is the closest constant from $?c2$, $?p2$ and $?b1$ while $C8$ is the closest one from $?c1$ and $?p1$.

Later, our experiments will show that this way of computing upper bounds provides reasonably good bounds in practice.

5.3 Choosing Partial PM-queries

Given a PM-query PQ , the problem of choosing a partial PM-query $PPQ = opt(PQ)$ for it is that of ensuring that mapping the variables of PPQ against $\mathcal{G}$ results in maximizing $sub^*(PQ\theta)$ where θ is an answer substitution for PPQ . In other words, we want to define function opt in such a way that $sub^*(PPQ, PQ) = \prod_{?x \in (V_{PQ} \setminus V_{PPQ}) \cap VAR} cand^*(PQ, ?x)$, which is the upper bound on the number of substitutions for the variables in PQ that were not chosen as variables of PPQ , is maximized.⁸

We first show that the problem of computing $opt(PQ)$ is NP-hard, then we propose two approaches for addressing it.

To show NP-hardness of $opt(PQ)$, we start by introducing a decisional variant $opt(PQ)_{log}^B$ defined as the problem of deciding whether there is a partial PM-query PPQ for PQ such that $\log_2 sub^*(PPQ, PQ) \geq B$.⁹ Theorem 5.7 characterizes the complexity of this variant.

THEOREM 5.7. $opt(PQ)_{log}^B$ is NP-complete.

Now, it is easy to observe that $opt(PQ)_{log}^B$ can be polynomially decided after solving the original problem $opt(PQ)$. Indeed, $opt(PQ)_{log}^B$ is true iff $opt(PQ)$ returns a partial PM-query PPQ such that $\log_2 sub^*(PPQ, PQ) \geq B$. Thus, $opt(PQ)$ is NP-hard.

To compute $opt(PQ)$ we propose two alternative approaches: a list-oriented pruning method and a reduction to the NWST problem.

List-Oriented Pruning. Given a PM-query PQ , a partial PM-query for PQ can be generated by choosing a set $V_s \subset V_{PQ}$, and then checking whether Definition 5.1 holds for the partial PM-query induced by the vertices in V_s (denoted $PQ(V_s)$). The list-oriented pruning method starts by building the list of all subsets V_s of V_{PQ} s.t. $|V_s| = |V_{PQ}| - 1$. Then, the list is processed as follows. For each unprocessed subset V_s in the list, if $PQ(V_s)$ satisfies Definition 5.1, then the algorithm adds all the subsets of V_s with cardinality $|V_s| - 1$ to the list—otherwise, V_s is immediately pruned from the list. When all the subsets in the list have been processed, the algorithm selects the one for which $sub^*(PQ(V_s), PQ)$ is maximum. It is easy to see that if V_s does not comply with Definition 5.1, then no subset of V_s can do: (i) if $\mathcal{E}(PQ) \not\subseteq V_s$, then we have $\mathcal{E}(PQ) \not\subseteq V'_s$ for any $V'_s \subset V_s$; (ii) if a path between the essential variables of PQ , or between an essential variable and a constant vertex, cannot be defined using the vertices in V_s , then no path can be defined using any subset of V_s .

⁸The reason why we want to maximize $sub^*(PPQ, PQ)$ is related to how pruning is applied. Intuitively, during query processing, if we pick the vertices that will possibly get a higher exact score, we increase the chances that more vertices will drop below the current threshold. Further details are provided in Section 5.4.

⁹For technical reasons, we use log. It allows us to consider B such that its size is polynomial w.r.t. $|V_{PQ}|$ in the reduction of Theorem 5.7.

For instance, if we consider PQ_2 of our running example, $V_s = \{C7, ?b1, ?c2, ?p2\}$ does not comply with Definition 5.1 because $?c1$ is a scoring variable, so the algorithm avoids listing all of its subsets.

Reduction to the NWST Problem. The second approach reduces our problem to the NWST problem and then uses well-known approximate algorithms for NWST to compute (sub)optimal partial PM-queries. The NWST problem is defined as follows. Given an undirected graph $\widehat{G} = \langle \widehat{V}, \widehat{E} \rangle$, a node-weight function $\omega : \widehat{V} \rightarrow \mathbb{N}$, and a subset of vertices $S \subseteq \widehat{V}$ (called *terminals*), compute the minimum weight subtree of $\widehat{G}$ that includes all the vertices in S .

We reduce the problem of computing $opt(PQ)$ to an instance $NWST(PQ)$ of NWST as defined below.

Definition 5.8 (NWST(PQ)). Given a PM-query $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$, an instance $NWST(PQ)$ of NWST is defined as follows: (i) $\widehat{V}$ contains the same vertices as PQ ; (ii) $\widehat{E}$ contains an undirected edge (v_1, v_2) for each edge $(v_1, \{\ell\}, 1, v_2)$ or $(v_2, \{\ell\}, 1, v_1)$ in E_{PQ} ; (iii) $S = \mathcal{E}(PQ) \cup (V_{PQ} \cap V)$, i.e., S consists of all the essential variables and constant vertices of PQ ; (iv) $\forall v \in S, \omega(v) = 0$ and $\forall x \in \widehat{V} \setminus S, \omega(v) = \ln cand^*(PQ, ?x)$.

It turns out that solving $NWST(PQ)$ suffices to solve $opt(PQ)$.

THEOREM 5.9. *Given a PM-query PQ , every solution T of $NWST(PQ)$ one-to-one corresponds to a partial PM-query $PPQ(T)$ for PQ such that $sub^*(PPQ(T), PQ)$ is maximum.*

Thus, many well-known approximate algorithms for NWST can be used to compute $opt(PQ)$. For instance, Reference [21] presents two algorithms with $1.35 \ln |S|$ and $1.65 \ln |S|$ as the worst-case approximation ratios. Interestingly, these approximation ratios do not depend on the size of the graph but only on the number of terminal vertices, which corresponds in our case to the number of constant vertices and essential variables. In our implementation, we used the faster $1.65 \ln |S|$ algorithm.

5.4 The PScore Algorithm

We conclude the section by showing how the various techniques described in the previous sections fit together in our overall query-processing algorithm, named PScore (Algorithm 1).

The algorithm, on Line 5, applies one of the two optimization methods described in Section 5.3. If the list-oriented pruning method is applied, we call the algorithm PScore_LP; otherwise, we call it PScore_NWST.

The computation of exact scores (Lines 12 and 20) is done by trying to extend every partial substitution θ associated with a vertex in T to a “full” substitution (i.e., by computing an answer substitution for $PQ_i\theta$ if θ is an answer substitution for PPQ_i). To achieve this, the algorithm employs the *map* algorithm described in Section 6.2.

It should be observed that:

- The algorithm prunes away all vertices in the table *whose upper bound is less than or equal to the exact score of the k -th result*, by comparing this score with the maximum upper bound of the unprocessed vertices (Lines 15–19).
- The algorithm gracefully handles negative scores and anti-monotonic range-closed functions thanks to the use of essential partial substitutions. In fact, the upper bounds computed for the vertices in T are independent of whether scoring terms may produce negative scores or aggregation functions are anti-monotonic—upper bounds are “automatically” kept correct by the fact that range-closed aggregation functions are guaranteed to keep their values in the expected range.

ALGORITHM 1: PScore

```

1: procedure PSCORE( $S$ -query  $SQ = \langle PQS, ga \rangle$ )
2: data structure: Candidate output table  $T$ 
3: data structure: Set  $ans$  containing  $k$  vertices along with their exact scores
4: for every  $PQ_i \in PQS$  do
5:    $PPQ_i \leftarrow opt(PQ_i)$ 
6:   compute all answer substitutions for  $PPQ_i$ 
7:   initialize  $T$  using the substitutions obtained at Line 6
8:   for every vertex  $v$  in  $T$  do
9:     compute  $score^*(v)$ 
10:   $H \leftarrow$  the  $k$  vertices in  $T$  having the higher upper bounds
11:  for every  $v \in H$  do
12:    compute  $score(v, SQ)$ 
13:   $ans \leftarrow H$ 
14:  while  $T$  is not empty do
15:     $v \leftarrow$  vertex with maximum  $score^*(v)$  in  $T$ 
16:    remove  $v$  from  $T$ 
17:     $v_k \leftarrow$  vertex in  $ans$  with minimum score
18:    if  $score^*(v) \leq score(v_k, SQ)$  then
19:      end procedure
20:    compute  $score(v, SQ)$ 
21:    if  $score(v, SQ) > score(v_k, SQ)$  then
22:      replace  $v_k$  with  $v$  in  $ans$ 
23: end procedure

```

—The algorithm proceeds in decreasing order of upper bounds because of the way vertices in the table are pruned. If the condition on Line 21 is true, then a vertex v has an exact score that makes it part of the current top- k answer. When this happens, the upper bounds of one or more vertices in the table drop below the current threshold—such vertices are “automatically” pruned as explained above. It can easily be observed that the higher the score of v , the higher the likelihood that a larger set of vertices will be pruned.

PROPOSITION 5.10. *Given an S -query $SQ = \langle PQS, ga \rangle$, the PScore algorithm terminates and correctly computes $ans(SQ)$. Its worst-case asymptotical time complexity is $O(T_{map} \cdot |V|^M)$ where $M = \max_{PQ \in PQS} |V_{PQ} \cap VAR|$ and T_{map} is the complexity of the map algorithm.*

Finally, it should also be observed that the PScore algorithm assumes the existence of at least k full substitutions—this is because Definition 4.6 requires $|ans(SQ)| = k$. However, the algorithm can be easily adapted to the case where the number of substitutions is lower than k and thus no top- k answer must be returned. In fact, it suffices to check that T (resp., ans) contains at least k vertices along with their scores after Line 7 (resp., Line 13) and end the procedure otherwise.

6 MANAGING EDGE-ANNOTATED QUERIES

In this section, we discuss how we extend the techniques presented in Section 5 to handle the case of edge-annotated PM-queries. In particular, Section 6.1 shows our approach to the computation of upper bounds and Section 6.2 describes the algorithm for computing substitutions.

Fig. 4. Expanded queries for PQ_2 of Figure 1. Fig. 5. Two partial PM-queries for PQ_2 .

6.1 Computing Upper Bounds on Scores

The computation of upper bounds for edge-annotated queries can take advantage of specific relationships among partial substitutions that are present in this case.

Consider for instance PQ_2 of our running example. An upper bound for it could be computed by (1) expanding it into an equivalent set $eq(PQ_2) = \{EQ_1, EQ_2, EQ_3, EQ_4\}$ (shown in Figure 4) of non-annotated “expanded” PM-queries for PQ , (2) processing such expanded queries one-by-one, and then (3) taking the sum of the resulting upper bounds (since the set of substitutions for PQ_2 is the union of the sets of substitutions for the expanded queries).

However, this would require processing a partial PM-query for each expanded query, and the number of expanded queries grows very quickly. Consider an edge-annotated PM-query $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$. For each annotated edge $e_i = (v_i, L_i, w_i, v'_i)$ in E_{PQ} , let $exp(e_i)$ be the set of edges $\{(v_i, L_i, 1, v'_i), (v_i, L_i, 2, v'_i), \dots, (v_i, L_i, w_i, v'_i)\}$. Now, observe that each expanded query in $eq(PQ)$ contains a different set of edges from $exp(e_1) \times \dots \times exp(e_n)$ where n is the number of annotated edges in E_{PQ} . Thus, there are $\prod_{i \in [1..n]} w_i$ expanded queries for PQ .

We therefore propose a different approach that heuristically chooses a set of partial PM-queries such that by extending a substitution for one of them, we can obtain full substitutions for more than one expanded query.

Example 6.1. By extending an essential partial substitution for $PPQ_{2,1}$ in Figure 5 (resp., $PPQ_{2,2}$), full substitutions for EQ_1 and EQ_2 (resp., EQ_3 and EQ_4) can be built. Now, suppose we compute a

substitution θ_1 for $PPQ_{2,1}$. This substitution will not map variables $?p1$ and $?p2$ of EQ_1 and variables $?p1$, $?p2$, and $?x$ of EQ_2 . The upper bound on the number of substitutions obtainable by extending θ_1 is therefore $sub^*(EQ_1\theta_1) + sub^*(EQ_2\theta_1) = cand^*(EQ_1\theta_1, ?p1) \times cand^*(EQ_1\theta_1, ?p2) + cand^*(EQ_2\theta_1, ?p1) \times cand^*(EQ_2\theta_1, ?p2) \times cand^*(EQ_2\theta_1, ?x)$. The same applies to any substitution θ_2 for $PPQ_{2,2}$: its upper bound is $sub^*(EQ_3\theta_2) + sub^*(EQ_4\theta_2) = cand^*(EQ_3\theta_2, ?p1) \times cand^*(EQ_3\theta_2, ?p2) + cand^*(EQ_4\theta_2, ?p1) \times cand^*(EQ_3\theta_2, ?p2) \times cand^*(EQ_4\theta_2, ?x)$.

In general, let PQ be a PM-query and PPQ a partial PM-query for it. Moreover, let $cov(PPQ) \subseteq eq(PQ)$ be the set of expanded queries such that by extending a substitution for PPQ , we obtain full substitutions for all the queries in $cov(PPQ)$ —for instance, in our example we have $cov(PPQ_{2,1}) = \{EQ_1, EQ_2\}$. Given a substitution θ for PPQ , we have $sub^*(PQ\theta) = \sum_{EQ \in cov(PPQ)} sub^*(EQ\theta)$.

We now describe our heuristics to choose a set Q of partial PM-queries for an edge-annotated PM-query PQ . Obviously, Q must “fully cover” the set of expanded queries for PQ , that is, it must satisfy $\cup_{PPQ \in Q} cov(PPQ) = eq(PQ)$. To ensure this, and to possibly provide high-quality partial PM-queries, we first build a modified version PQ' of PQ (by replacing annotated edges with non-annotated ones), then we compute $opt(PQ')$ and use the result to compute Q .

Set $E_{PQ'}$ is built from E_{PQ} by replacing each annotated edge $e = (v, L, w, v')$ with two edges $mod_1(e) = (v, L, 1, ?V)$ and $mod_2(e) = (?V, L, 1, v')$ with $?V$ being an artificial variable not in V_{PQ} —the number of such new edges is $2n$, i.e., twice the number of annotated edges in E_{PQ} . Now, to compute $PPQ' = opt(PQ')$ we need to choose a good value for $cand^*(PQ', ?V)$ —this value cannot be derived from the PM_Index as $?V$ is an artificial variable we introduce just for dealing with annotated edges. Consider the “longest expansion” of e that consists of the following path of w non-annotated edges: $(v, L, 1, ?V_1), (?V_1, L, 1, ?V_2), \dots, (?V_{w-1}, L, 1, v')$ with each $?V_i$ being an artificial variable not in V_{PQ} . We define $cand^*(PQ', ?V)$ as $\frac{1}{|eq(PQ')|} \sum_{i \in [1..w]} \sum_{j \in [1..|eq(PQ')|]} cand^*(EQ_j, ?V_i)$. Observe that due to the properties of the problem of choosing optimal partial PM-queries, function opt will either include both edges $mod_1(e)$ and $mod_2(e)$ in PPQ' , or none of them. The final set Q can then be computed from PPQ' as follows. For each annotated edge $e_i = (v_i, L_i, w_i, v'_i)$ in E_{PQ} , we define a set of edges $E_Q(e_i)$ as $exp(e_i)$ if $mod_1(e_i)$ is in PPQ' , and $\emptyset$ otherwise. Now we consider the set $EC = E_Q(e_1) \times \dots \times E_Q(e_n)$. Set Q is initialized with $|EC|$ partial PM-queries, containing only the non-annotated edges in E_{PQ} . Each of these queries is then extended with a different set of edges from EC . Observe that $|Q| = |EC| = \prod_{i \in [1..n], mod_1(e_i) \text{ in } PPQ'} w_i$. It is easy to see that this approach ensures that Q covers the set of expanded queries for PQ .

For instance, in our running example, if $opt(PQ_2)$ is a partial PM-query of the form $?c1 \leftarrow ?b1 \rightarrow ?c2 \ \& \ C8 \rightarrow ?c1 \leftarrow ?c2 \leftarrow C7$, then the final partial PM-queries are those reported in Figure 5.

As our experiments will show, this approach chooses good-quality partial PM-queries. Moreover, the structure of the *map* algorithm presented in Section 6.2 allows us to exploit commonalities between the queries in Q . In fact, the actual set of queries *map* must run over can just include the edges with the maximum-length annotation (i.e., (v_i, L_i, w_i, v'_i) in set $E_Q(e_i)$ above). The number of such queries is $|\{e_i \text{ in } PQ' \mid mod_1(e_i) \text{ in } PPQ'\}|$. In our running example, the input to the *map* algorithm would be the single partial PM-query $?c1 \leftarrow ?b1 \rightarrow ?c2 \ \& \ C8 \rightarrow ?c1 \xrightarrow{2} ?c2 \leftarrow C7$.

6.2 Mapping Algorithm

Algorithm 2 computes all answer substitutions for a given (edge-annotated) PM-query PQ against the graph database $\mathcal{G}$.

The algorithm essentially performs a depth-first search and, when it finds an edge e with an annotation greater than 1 (denoted $ann(e) > 1$) it starts a separate depth-first search using a copy of the query obtained by decreasing the annotation by 1. In the algorithm, S is the set of substitutions

being computed. Moreover, the algorithm uses an external function $mcand(u, L, ?v)$ that returns the set of vertices of $\mathcal{G}$ that can be matched to $?v$, i.e., those that are directly connected to u through an edge with a label in L . Note that $|mcand(u, L, ?v)|$ can be retrieved from the PM_Index. Access to graph data on disk is managed through the DOGMA index [7].

ALGORITHM 2: *map*

```

1: procedure map(PM-query  $PQ$ )
2:    $S \leftarrow \emptyset$ 
3:   if all vars are mapped and all edges' annotations are 1 then
4:     add the mapping of  $PQ$  to  $S$ 
5:   return  $S$ 
6:   if  $\exists(c_1, L, c_2)$  in  $PQ$  with  $ann(PQ, (c_1, L, c_2)) \geq 2$  then
7:      $PQ' \leftarrow PQ$ 
8:      $ann(PQ', (c_1, L, c_2)) \leftarrow 1$ 
9:     if  $(c_1, L, c_2)$  matches  $\mathcal{G}$  then
10:      add the result of map( $PQ'$ ) to  $S$ 
11:      $PQ'' \leftarrow PQ$  after removing  $(c_1, L, c_2)$ 
12:     add  $(c_1, L, ?x)$  to  $PQ''$ 
13:      $ann(PQ'', (c_1, L, ?x)) \leftarrow 1$ 
14:     add  $(?x, L, c_2)$  to  $PQ''$ 
15:      $ann(PQ'', (?x, L, c_2)) \leftarrow ann(PQ, (c_1, L, c_2)) - 1$ 
16:     add the result of map( $PQ''$ ) to  $S$ 
17:   else
18:      $(u, L, ?v) \leftarrow$  edge that minimizes  $|mcand(u, L, ?v)|$ 
19:     (always prefer edges with annotations equal to 1)
20:     for  $c \in mcand(u, L, ?v)$  do
21:        $PQ' \leftarrow PQ$ 
22:       substitute  $?v$  with  $c$  in all edges of  $PQ'$  that contain  $?v$ 
23:        $ann(PQ', (u, L, c)) \leftarrow 1$ 
24:       if all mapped edges of  $PQ'$  with  $ann = 1$  match  $\mathcal{G}$  then
25:         if  $\chi$  is satisfied after substituting  $?v$  with  $c$  then
26:           add the result of map( $PQ'$ ) to  $S$ 
27:       if  $ann(PQ, (u, L, ?v)) \geq 2$  then
28:          $PQ'' \leftarrow PQ$  after removing  $(u, L, ?v)$ 
29:         add  $(u, L, c)$  to  $PQ''$ 
30:          $ann(PQ'', (u, L, c)) \leftarrow 1$ 
31:         add  $(c, L, ?v)$  to  $PQ''$ 
32:          $ann(PQ'', (c, L, ?v)) \leftarrow ann(PQ, (u, L, ?v)) - 1$ 
33:         add the result of map( $PQ''$ ) to  $S$ 
34:   return  $S$ 
35: end procedure

```

In the algorithm, Lines 6–16 deal with the case of fully mapped edges with an annotation greater than 1, whereas Lines 18–33 deal with unmapped edges. In the first case, given an edge e to process, we create a copy PQ' of PQ with $ann(e) = 1$, and call *map*(PQ') recursively to continue its mapping (we call this the “Branch” operation). We also create a PQ'' where e is expanded to two edges whose annotations are 1 and $ann(e) - 1$, respectively, and call *map*(PQ'') recursively (“Spawn” operation). In the second case, we have to select one unmapped edge to find substitutions for (Line 18). We select the edge $(u, L, ?v)$ for which the number of vertices that can be matched to $?v$ is minimized.

(a) Graph database

(b) Branch and spawn operations

Fig. 6. Example graph database (a) and execution of the *map* algorithm up to the second level of recursion (b).

Then, for each vertex $c \in mcand(u, L, ?v)$, we create PQ' and PQ'' as we did in the first case, and call *map* recursively.

Subgraph isomorphism is checked on Lines 9 and 24. It should be noted that, until there is no mapped edge with annotation greater than 1, the processing of unmapped edges is deferred. We made this choice to maximize the chance to prune a branch on Line 9. It should also be observed that any SPARQL engine or subgraph matching algorithm could be used to check subgraph isomorphism—in our implementation we used the algorithm proposed for the DOGMA index [7].

Example 6.2. Consider the graph database in Figure 6(a) and the PM-query at the left of Figure 6(b). The algorithm starts by processing $C1 \xrightarrow{follows(2)} ?a$. A1 is the only neighbor of C1. For the branch operation, the algorithm substitutes $?a$ with A1. For the spawn operation, it expands the edge and substitutes the intermediate variable with A1. Note that expanded edges have annotations equal to 1 and $ann(C1 \xrightarrow{follows(2)} ?a) - 1 = 1$, respectively. After branching, $C2 \xrightarrow{follows(2)} A1$ is processed. In this case, for the branch operation the algorithm checks whether C2 and A1 are connected through *follows* in $\mathcal{G}$. If so, we have found an answer substitution (case 1. in the

Table 6. Graph Databases (Top) and Query Types (Bottom). In the Table, n_V is the Number of Vertices in Each PM-query ($|V_{PQ}|$), n_E the Number of Edges ($|E_{PQ}|$), and n_C the Number of Constant Vertices ($|V_{PQ} \cap V|$)

	$ V $	$ E $		$ V $	$ E $
Nuclear [1]	74K	1.1M	Flickr [9]	6.2M	15.2M
CiteSeerX [13]	0.93M	2.9M	BSBM [6]	14.4M	37.2M
IMDb [25]	2.1M	7.7M	Orkut [33]	3.7M	234M
YouTube [12]	4.6M	14.9M			

	Small tree			Small graph			Large tree			Large graph		
	n_V	n_E	n_C	n_V	n_E	n_C	n_V	n_E	n_C	n_V	n_E	n_C
Nuclear	5	4	1	5	8	1	10	9	4	10	15	4
CiteSeerX	5	4	1	5	8	1	10	9	4	10	15	4
IMDb	5	4	2	–	–	–	9	8	4	–	–	–
YouTube	6	5	1	6	10	1	10	9	3	10	15	3
Flickr	5	4	1	5	6	1	10	9	4	10	11	4
Orkut	5	4	2	5	8	2	10	9	5	10	15	5

figure). For the spawn operation, an intermediate variable $?x$ is added and the mapping continues. The process goes on until all substitutions (such as cases 1 and 5 in the figure) are found.

PROPOSITION 6.3. *Given a PM-query PQ , Algorithm 2 terminates and correctly computes all answer substitutions for PQ in time $O(|eq(PQ)| \cdot |V|^{|\mathcal{V}_{PQ} \cap \mathcal{V}_{AR}| + v})$, where $v = \sum_{(v, S, w, v') \in E_{PQ}} (w - 1)$.*

7 EXPERIMENTAL EVALUATION

7.1 Setting

We tested our framework using the seven graph databases in Table 6. For all databases but BSBM, we generated 3K S-queries, each containing three PM-queries. In turn, for each PM-query, we started by randomly retrieving a connected subgraph (or subtree) from the database with a fixed number of vertices and edges. We then replaced a fixed portion of the vertices with variables. We generated four different types of queries, whose numbers of vertices, edges, and constant vertices are reported in Table 6.¹⁰ For the IMDb database, which is mostly tree-structured, we only built tree-structured queries. For the BSBM dataset, we used a modified version of the six test queries in Reference [32], to which we added GROUP BY statements and anchors to create aggregate top- k queries.

To vary the selectivity of the queries, we used a parameter $\gamma \in \{0.3, 0.7\}$ that represents the percentage of variables with constraints (i.e., variables for which function ϱ of Definition 4.1 is defined)—for a variable $?v$ that replaced a vertex u with property $u.p = z$, we wrote a constraint whose form is either $?v.p \geq z$ or $?v.p \leq z$ (if u had multiple numerical properties, we chose one randomly). This way, we also guaranteed that there exists at least one substitution for each query (we actually obtained up to tens of millions of substitutions). Moreover, for each query, we

¹⁰For other works that use similar approaches to the selection of queries, see, e.g., References [6, 37, 39, 49].

randomly chose a subset of variables and designated them as output variables (up to 50%, with an average of 25%). Functions *la* and *ga* were chosen randomly as well.

We generated queries by starting from a group of 1K S-queries containing only non-annotated PM-queries with single labels on all edges. We then generated 1K annotated S-queries by randomly adding annotations to edges: 60% of edges had $w = 1$, 25% had $w = 2$, 10% had $w = 3$, and 5% had $w = 4$.¹¹ Finally, we generated 1K annotated multiple-label S-queries by adding further labels on 40% of the edges.

We evaluated the performance of PScore_LP and PScore_NWST with different query types and values of γ . We compared our algorithms with (i) a PScore_Base algorithm that computes all answers to the query, scores them, and selects the top- k ,¹² and (ii) two of the most popular RDF query engines, Jena [8, 26, 51] and GraphDB [5, 19] (formerly known as OWLim). We point out that none of these systems is specifically targeted at aggregate top- k computation, whereas we apply a specialized approach to the problem—thus, we expected our algorithms to outperform such systems. Moreover, GraphDB strictly adheres to the SPARQL 1.1 standard, where path edges cannot have length constraints—thus, we tested GraphDB by first expanding each annotated PM-query PQ into its equivalent set of non-annotated queries $eq(PQ)$ as described in Section 6.1. Finally, Jena supports path edges with limited path length as we do in our PM-queries, but it suffers from the limitations discussed in Section 2.

All the experiments were run on a Xeon 5140 CPU clocked at 2.33GHz, equipped with 16GB RAM and running RedHat Linux.

7.2 Results

In a first round of experiments, we measured the query evaluation times obtained with $k = 10$ using annotated single-label queries. The results are reported in Figure 7.

The evaluation times we obtained are very satisfactory in general. On all datasets but IMDB, the performance advantage of PScore_Base over GraphDB ranges between 35.8% and 75.8%, with an average of 58.4%. The only cases where PScore_Base and GraphDB show similar performance are those involving tree-structured queries on the IMDB dataset. Jena was not able to complete the query evaluation process in over half the cases (for each query, we fixed a timeout equal to 4 times the query evaluation time of PScore_Base) except for the BSBM dataset. The percentage of timeouts w.r.t. the total number of queries of a certain type/size/selectivity (see Table 7) was up to 90.5%. Interestingly, the percentage of timeouts decreased around 20% on average when we used equivalent sets of non-annotated queries.

In addition, PScore_LP and PScore_NWST largely outperform PScore_Base on all datasets. The performance advantage ranges between 53.7% and 95.8%, with an average of 75.8%. This is mainly a consequence of the much smaller number of full substitutions PScore_LP and PScore_NWST need to compute. Figure 8 reports statistics about the average percentage of substitutions they processed w.r.t. PScore_Base during this round of experiments. The results show that both the algorithms save over 60% in the majority of cases, and over 90% in more than 30% of cases.

Generally, the relative performance of PScore_LP and PScore_NWST depends on the query type. In small tree queries, the quality of the partial PM-queries computed by PScore_NWST is very close to that obtained by PScore_LP, while requiring shorter computation times. In small graph queries, the advantage provided by PScore_LP's better partial PM-queries appears to

¹¹We recall that w is the integer value associated with annotated edges (Definition 4.1). Connections involving more than four edges have been shown to have very limited usefulness in practical scenarios [2].

¹²It should be observed that, although the PScore_Base algorithm does not apply any kind of pruning over the set of substitutions, it still benefits from the efficient disk access employed by the *map* algorithm.

Fig. 7. Query evaluation time for different algorithms, values of γ , and query types—label A/x means algorithm A with $\gamma = x$.

Table 7. Percentage of Jena Timeouts

γ	Small tree	Small graph	Large tree	Large graph
0.3	59.4%	79.4%	76.6%	88%
0.7	61.4%	81%	83.7%	90.5%

Fig. 8. Average percentage of substitutions processed by PScore_LP and PScore_NWST w.r.t. PScore_Base.

compensate for its longer computation time. In large tree and large graph queries, PScore_LP takes much longer to compute the partial PM-queries, and their better quality appears to have less impact than the longer computation times. *Wrapping up*, PScore_NWST appears to be the best choice for tree-structured and larger queries, whereas PScore_LP is better suited for small graph queries. Interestingly, in the majority of cases the performance advantage of PScore_NWST over PScore_LP slightly increases (around 2%) when $\gamma = 0.7$.

Moreover, we specifically assessed the benefits provided by the use of the PM_Index as well as the quality of the upper bounds computed using the index, as described in Section 5.2. Figure 9 shows the performance advantage obtained when we precompute the PM_Index (which is the default case in this experimental assessment) w.r.t. the case where the information provided by the index is computed on-the-fly. The results confirm noticeable benefits: the advantage is around 17.5% on average, and more than 30% in some cases on the CiteSeerX, IMDb, YouTube, and Flickr datasets.

Figure 10 shows that the ratios between upper bounds and real scores of the substitutions processed are satisfactory (under 1.5 in the majority of cases).

In addition, to verify that the PScore algorithm quickly finds out that there is no top- k answer to be returned when the number of substitutions is lower than k (as discussed in Section 5.4), we ran a modified version of the queries on the Orkut dataset. In these queries, we replaced a constant with one that is not present in the dataset—the other parameters were those used for the original experiments (Figure 7). Evaluation times were indeed extremely low, never exceeding 2 seconds. As expected, PScore_NWST was faster than PScore_LP as it saved additional time when computing partial PM-queries.

Our second round of experiments (Figure 11) assessed how the performance of PScore_NWST and PScore_LP varies with the value of k . We measured query evaluation times obtained for different values of k and γ , using annotated single-label queries. As expected, since pruning happens later when k increases, evaluation times increase with k . Both our algorithms scale gracefully with k , and PScore_NWST is faster than PScore_LP in the majority of cases with $\gamma = 0.3$ and in all cases

Fig. 9. Performance advantage with precomputation of the PM_Index.

Fig. 10. Average ratio between upper bounds and real scores of the substitutions processed by PScore_LP and PScore_NWST.

with $\gamma = 0.7$. PScore_Base, GraphDB and Jena do not prune, so their times cannot vary significantly w.r.t. k —on average, the performance advantage of PScore_NWST over GraphDB was 85.1%.

In a third round of experiments, we assessed how the performance of PScore_NWST varies w.r.t. different query groups (non-annotated/single-label, annotated/single-label, annotated/multiple-label). The results we obtained with $k = 10$ on the Flickr dataset (that is the largest dataset with multiple labels for which we built synthetic queries) are reported in Figure 12. As expected, the impact of adding annotations and multiple labels is higher when $\gamma = 0.3$, due to the higher number of substitutions the algorithm must handle.

Finally, we also measured the size and the build time of the PM_Index for different values of maximum distance. The results are reported in Table 8.¹³ Here, we can observe that the size of the index (whose increase w.r.t. distance depends on the average distance between vertices) “stabilizes” at a value of maximum distance around 3. Build times appear satisfactory if we consider the size of the datasets¹⁴ and, more importantly, the fact that the PM_Index (if used) is likely to be built in an offline fashion.

7.3 Quality of the Answers

We performed additional experiments to assess the quality of the answers provided by our framework, as perceived by human users.

We provided 10 users with an anonymized version of the Nuclear dataset and asked them to express their preferences about the answers computed using (1) our query model, (2) a model that finds top- k substitutions based on a user-defined scoring function and does not perform aggregations (such as those in References [32, 39]),¹⁵ and (3) a model that performs inexact matching based on wildcards or multivalued attributes (such as that in Reference [41]).

To achieve this, we defined the following five questions and translated them into queries in each query model (a graphical representation of the S-queries obtained this way is reported in the Appendix). For each question, the users were asked to evaluate the quality of the results by stating their preferences with respect to the three top-five answer sets computed using the above query models.

Q_1 Which member of a given very large terrorist group has the most significant connections to other suspicious individuals?

¹³ $h \geq 4$ was not needed for the BSBM queries.

¹⁴In particular, the construction of the PM_Index has shown an approximate average case complexity of $O(|E|)$ in our experiments.

¹⁵This model actually corresponds to the SPARQL query model with ORDER BY.

Fig. 11. Query evaluation time for different algorithms and values of k and γ .

- Q_2 Which of a given holding company's partner companies has the most significant connections with other suspicious individuals or companies?
- Q_3 Which company has the most significant connections with a given terrorist who is a primary suspect in a well-known attack, and to his friends?
- Q_4 Who is the key person connecting a given government intelligence agency, which has a large number of connections to many individuals, with other government agencies?

Fig. 12. Query evaluation time for different query groups and values of γ . Label $X/Y/x$ means query group X/Y with $\gamma = x$. Annotated (resp. non-annotated) queries are denoted as A (resp. NA). Single-label (resp. multiple-label) queries are denoted as SL (resp. ML).

Table 8. Size (Number of Rows) and Build Time of the PM_Index for Different Values of Maximum Distance

	1	2	3	4	5	Time
Nuclear	0.52M	0.9M	1.29M	1.5M	2.38M	5 mins
CiteSeerX	2.15M	3.94M	5.17M	5.84M	6.08M	8 mins
IMDb	2.51M	8.81M	14.02M	22.31M	24.46M	40 mins
YouTube	5.94M	9.95M	11.25M	11.31M	11.31M	19 mins
Flickr	8.94M	23.60M	35.06M	35.74M	36.04M	59 mins
BSBM	30.33M	109.72M	151.62M	—	—	28 mins
Orkut	24.1M	96.89M	110.01M	112.34M	114.2M	78 mins

Fig. 13. User-perceived quality of the answers provided by our framework.

Q_5 Which company among all those connected to a given banking company in Asia has the most significant connections to suspicious individuals?

Figure 13 summarizes how the results computed using our proposed query model were ranked. In particular, for each query, the figure reports the number of users that stated that the answer set provided by our framework was their first, second, or third choice.

The results appear very satisfactory. In 32 out of 50 cases, our query model was identified as the one that provides the best answers (first choice)—in 12 cases, it was ranked as the second choice. In addition, (i) for all queries but Q_5 , at least half of the users stated that our model was their first choice and (ii) for all queries, at least seven users stated that our model was their first or second choice.

It should also be observed that, in general, the perceived quality of the answers also depends on the specific way natural-language questions are translated into graph queries. In our experiments, the users were only made aware of the questions and then looked directly at the results (not at the actual graph queries). For instance, if we consider Q_5 —“Which company among all those connected to a given banking company in Asia has the most significant connections to suspicious individuals?”—the corresponding graph-based query captures just one specific way of defining “significant connections.” We believe that, with an in-depth knowledge of the application domain, and possibly after exchanging information with the users about the specific semantics of the questions they are interested in, the perceived quality of the answers can be further improved.

8 CONCLUSIONS

Edge-labeled graphs are occurring increasingly frequently. In many applications, it is appropriate to allow a user to specify functions that capture what is important for her because any system-defined function would necessarily not take application-specific knowledge into account. For instance, how a nuclear proliferation expert assesses a vertex to be suspicious would differ from how an MIF investigator assesses a vertex’s level of suspicion. In this article, we argue that the user may express her notion of importance via a set of subgraph patterns called PM-queries, and propose two query processing algorithms that leverage the notion of “partial PM-queries.” We carried out detailed experiments with real-world graph databases with up to 234M edges. Our experiments show that answers on these real-world datasets can be computed in very good time frames.

APPENDICES

A PROOF OF THEOREM 5.5

Claim: Suppose $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$ is a PM-query. Then

$$sub^*(PQ) = \prod_{?x \in V_{PQ} \cap VAR} cand^*(PQ, ?x)$$

is an upper bound on the number of substitutions for PQ .

PROOF. We start by observing that any PM-query PQ can be decomposed into $h = |V \cap V_{PQ}|$ disjoint PM-queries $ST(c_1), ST(c_2), \dots, ST(c_h)$ such that each $ST(c_i)$ is a sub-tree of PQ rooted at constant vertex c_i (for simplicity, we do not consider χ and ϱ here). The set of answer substitutions for each $ST(c)$, denoted $\Theta(c)$, contains all the substitutions that can be obtained by projecting answer substitutions for PQ over the variables in $ST(c)$. Thus, an upper bound on the number of substitutions for PQ is $\prod_{c \in V \cap V_{PQ}} |\Theta(c)|$.

Now, for each constant c , let VAR_c be the set of variables $?x$ that are closest to c and, therefore, whose $cand^*(PQ, ?x)$ values are assigned based on the shortest path between c and $?x$ (by definition of $cand^*(PQ, ?x)$). The set of shortest paths from c to each $?x \in VAR_c$ constitutes a tree rooted at c . If we use this tree as our $ST(c)$, an upper bound on $|\Theta(c)|$ can easily be computed by taking the product of the $cand^*(PQ, ?x)$ values of all variables in $ST(c)$. Thus, we can derive $\prod_{c \in V \cap V_{PQ}} |\Theta(c)| \leq \prod_{c \in V \cap V_{PQ}} \prod_{?x \in V_{ST(c)} \cap VAR} cand^*(ST(c), ?x) = \prod_{?x \in V_{PQ} \cap VAR} cand^*(PQ, ?x)$. The statement follows. $\square$

B PROOF OF THEOREM 5.7

Claim: $\text{opt}(PQ)_{\log}^B$ is NP-complete.

PROOF. Membership in NP is trivial. We show NP-hardness by reduction from the Steiner tree problem [17] defined as follows. Given an undirected graph $\widehat{G} = \langle \widehat{V}, \widehat{E} \rangle$ a subset of vertices $S \subseteq \widehat{V}$ called *terminals*, and a positive integer $K \leq |\widehat{V}| - 1$, decide whether there is a subtree of $\widehat{G}$ that includes all the vertices in S (i.e., a spanning tree for S) and contains no more than K edges. Given an instance of ST, we construct an instance of our problem as follows. Let $B = |\widehat{V}| - (K + 1)$, and $PQ = \langle V_{PQ}, E_{PQ}, \chi, \varrho, la \rangle$ be such that (i) V_{PQ} consists of a variable $?v$ for each vertex $v \in \widehat{V}$, plus an additional constant vertex c ; (ii) E_{PQ} consists of an edge $(?v_1, \{\ell\}, 1, ?v_2)$ for each edge $(v_1, v_2) \in \widehat{E}$, plus an additional edge $(?v^*, \{\ell\}, 1, c)$ where v^* is any vertex in S and ℓ is any edge label; (iii) χ is empty; (iv) $\forall v \in S \varrho(?v) = t$, where t is any numerical term; (v) la is any aggregation function. Moreover, assume that $\forall ?v \in V_{PQ}, \text{cand}^*(PQ, ?v) = 2$ (it can be easily shown that there always exist a graph database such that $\text{cand}(c, \delta, \pi, e) = 2$, where c is the constant vertex of PQ).

Observe that each variable $?v$ corresponding to a vertex $v \in S$ is associated with a numerical term by ϱ , so $?v$ is an output variable of PQ , and thus it belongs to the set of essential variables, i.e., $\mathcal{E}(PQ) = \{?v \mid v \in S\}$.

We now show that there is a tree $T = \langle \widehat{V}_T, \widehat{E}_T \rangle$ of $\widehat{G}$ that includes all terminals and contains no more than K edges iff there is a partial PM-query PPQ for PQ such that $\log_2 \text{sub}^*(PPQ, PQ) \geq B$.

($\Rightarrow$) Given such a tree $T = \langle \widehat{V}_T, \widehat{E}_T \rangle$, we define $PPQ(T)$ such that $V_{PPQ(T)} = \widehat{V}_T \cup \{c\}$ and $E_{PPQ(T)} = \widehat{E}_T \cup \{(?v^*, \{\ell\}, 1, c)\}$. Clearly $PPQ(T)$ is a partial PM-query, as there exists at least one path between every pair of essential variables in $\mathcal{E}(PQ)$ (since there is one path in T between each pair of terminals), and at least one path between each essential variable in $\mathcal{E}(PQ)$ and the constant vertex $c \in V_{PPQ(T)}$ (in fact, c is connected to essential variable $?v^*$ by $(?v^*, \{\ell\}, 1, c) \in E_{PPQ(T)}$, and $?v^*$ is connected to the other essential variables of PQ). Moreover, $PPQ(T)$ is such that

$$|?v \in (V_{PQ} \setminus V_{PPQ(T)}) \cap \text{VAR}| = |\widehat{V}| - (K + 1). \text{ Thus, } \log_2 \left(\prod_{?x \in (V_{PQ} \setminus V_{PPQ(T)}) \cap \text{VAR}} \text{cand}^*(PQ, ?x) \right) = \sum_{?x \in (V_{PQ} \setminus V_{PPQ(T)}) \cap \text{VAR}} \log_2 \text{cand}^*(PQ, ?x) = |?x \in (V_{PQ} \setminus V_{PPQ(T)}) \cap \text{VAR}| \geq B.$$

($\Leftarrow$) Assume now that there is a partial PM-query PPQ for PQ such that $\log_2 \text{sub}^*(PPQ, PQ) \geq B$. Thus, there is subgraph $\langle V_{PPQ}, E_{PPQ} \rangle$ of $\langle V_{PQ}, E_{PQ} \rangle$ such that (i) $\{c\} \cup \mathcal{E}(PQ) \subseteq V_{PPQ}$, (ii) there is least one path between each essential variable in $\mathcal{E}(PQ)$, (iii) there is at least one path between each essential variable in $\mathcal{E}(PQ)$ and the constant vertex $c \in V_{PPQ}$, and (iv) $\log_2 \text{sub}^*(PPQ, PQ) = |?x \in (V_{PQ} \setminus V_{PPQ(T)}) \cap \text{VAR}| \geq B$. Let $G(PPQ) = \langle V(PPQ), E(PPQ) \rangle$ be the subgraph of $\widehat{G}$ such that $V(PPQ) = \{v \mid ?v \in V_{PPQ} \cap \text{VAR}\}$ and $E(PPQ) = \{(v_1, v_2) \mid (?v_1, \{\ell\}, 1, ?v_2) \in E_{PPQ} \text{ and } ?v_1, ?v_2 \in V(PPQ)\}$. Clearly, $|V(PPQ)| = |V_{PPQ} \cap \text{VAR}| \leq |V_{PQ} \cap \text{VAR}| - B = |\widehat{V}| - (|\widehat{V}| - (K + 1)) = K + 1$. Hence, if $G(PPQ)$ is a tree, we are done, since it is a subtree of $\widehat{G}$ that includes all vertices in S and contains no more than K edges. Otherwise, a spanning tree $T(PPQ)$ for the whole set of vertex $V(PPQ)$ of $G(PPQ)$ can be constructed in polynomial time by removing some edges from $E(PPQ)$. This way a subtree $T(PPQ)$ of $\widehat{G}$ that includes all terminals and contains no more than $K + 1$ vertices (and thus K edges) is obtained as well. $\square$

C PROOF OF THEOREM 5.9

Claim: Given a PM-query PQ , every solution T of $\text{NWST}(PQ)$ one-to-one corresponds to a partial PM-query $PPQ(T)$ for PQ such that $\text{sub}^*(PPQ(T), PQ)$ is maximum.

PROOF. Let T be a minimum weight subtree $T = \langle \widehat{V}_T, \widehat{E}_T \rangle$ of $NWST(PQ)$ such that T includes all the vertices in S . Let $PPQ(T)$ be such that $V_{PPQ(T)} = \widehat{V}_T$ and $E_{PPQ(T)} = \widehat{E}_T$.

Clearly, Definition 5.1 holds for $PPQ(T)$, as there is one path in T between each pair of vertices in $S = \mathcal{E}(PQ) \cup (V_{PQ} \cap V)$. Observe that $PPQ(T)$ includes all the constant vertices of PQ . However, the value $sub^*(PPQ(T), PQ)$ does not depend on this.

We now show that $sub^*(PPQ(T), PQ)$ is maximum. Let V^* be the set $V_{PPQ(T)} \cap VAR$. The fact that $\sum_{v \in V_T} \omega(v)$ is minimum entails that $\sum_{?x \in V^*} \omega(?x) = \sum_{?x \in V^*} \ln cand^*(PQ, ?x) = \ln \prod_{?x \in V^*} cand^*(PQ, ?x)$ is minimum too. Therefore, $\ln sub^*(PPQ(T), PQ) =$

$$\begin{aligned} & \ln \prod_{?x \in (V_{PQ} \setminus V_{PPQ(T)}) \cap VAR} cand^*(PQ, ?x) = \\ & \ln \frac{\prod_{?x \in V_{PQ} \cap VAR} cand^*(PQ, ?x)}{\prod_{?x \in V^*} cand^*(PQ, ?x)} = \\ & \ln \prod_{?x \in V_{PQ} \cap VAR} cand^*(PQ, ?x) - \ln \prod_{?x \in V^*} cand^*(PQ, ?x) \end{aligned}$$

is maximized, as the subtrahend is minimized. $\square$

D QUERIES USED IN SECTION 7.3

The queries used in the evaluation of the quality of the answers are reported below.

(a) Q_1

(b) Q_2

(c) Q_3

(d) Q_4

(e) Q_5

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Received May 2016; revised October 2017; accepted March 2018