

Counting to k , or how SPARQL1.1 Property Paths Can Be Extended to Top- k Path Queries*

Vadim Savenkov

Vienna University of Economics and Business
Welthandelsplatz 1
Vienna, Austria 1020
vadim.savenkov@wu.ac.at

Jürgen Umbrich

Vienna University of Economics and Business
Welthandelsplatz 1
Vienna, Austria 1020
juergen.umbrich@wu.ac.at

Qaiser Mehmood

Insight Centre for Data Analytics, NUI Galway
P.O. Box 1212
Galway, Ireland 43017-6221
qaiser.mehmood@insight-centre.org

Axel Polleres

Vienna University of Economics and Business and
Complexity Hub Vienna
Vienna, Austria
axel.polleres@wu.ac.at

ABSTRACT

While graph data on the Web and represented in RDF is growing, SPARQL, as the standard query language for RDF still remains largely unusable for the most typical graph query task: finding paths between selected nodes through the graph. Property Paths, as introduced in SPARQL1.1 turn out to be unfit for this task, as they can only be used for testing path existence and not even allow to count the number of paths between nodes. While such a feature has been shown to theoretically highly intractable, particularly in graphs with a high degree of cyclicity, practical use cases still demand a solution. A common restriction in fact is not to ask for all, but only the k -shortest paths between two nodes, in order to obtain at least the most important of potentially infeasibly many possible paths. In this paper, we extend SPARQL 1.1 property paths in a manner that allows to compute and return the k shortest paths matching a property path expression between two nodes. We present an algorithm and implementation and demonstrate in our evaluation that a relatively straightforward solution works (in fact, more efficiently than other, tailored solutions in the literature) in practical use cases.

CCS CONCEPTS

•Information systems →Network data models; Resource Description Framework (RDF); •Theory of computation →Shortest paths;

KEYWORDS

k shortest paths, SPARQL, querying RDF data, routing

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1 INTRODUCTION

RDF data on the Web is starting to form a constantly growing, labelled graph, sometimes called Linked Data, sometimes called the “Web of Data”, but anyway justifying the claim that a tangible portion of a “Semantic Web” has become a reality. In order to query RDF and Linked Data graphs, SPARQL as the standard query language is typically the tool of choice, but several omissions still make it far from perfectly fit for the task. For instance, while SPARQL 1.1 introduced a form of path queries to discover path existence between two nodes – this feature, called property paths – is not able to retrieve or count paths. In fact, there is a history behind this, as the seminal paper by Perez et al. in 2012, warned us not to “count beyond the Yottabyte”, i.e. the paper showed not only that – at that time current – SPARQL engines implemented property paths in an inefficient manner, but also that a query language feature that allowed to return (the number of) *all* property paths would become easily infeasible even in relatively small graphs with potentially double-exponential many solutions.

The existential semantics which the authors proposed to the rescue (and which became eventually a part of the final SPARQL 1.1 standard), yet has its limitations in practice where path existence alone is too limited for many practical cases, where also paths themselves are of interest. For instance, in professional social networks, typically everybody is (somehow) transitively connected to anyone, but we are interested in the k most promising connections to get introduced to some peer.

The SPARQL property path query

Listing 1: Property Path query in SPARQL1.1

```
SELECT * WHERE { :me foaf:knows+ :alice }
```

would not help here, in fact, it would simply return an empty binding. Likewise, for most practical routing applications the mere reachability test is not enough. On the other hand, enumerating or even simply counting all paths between given points is not required

either: rather, only the top most relevant (e.g., shortest) paths need to be found.

A particular interest for path queries comes from the bioinformatics domain where the volume of semantic data is constantly growing [4]. For instance, in the area of *cancer genomics* experts often need to discover relevant associations between biological and genetic entities such as diseases, drugs, genes, pathways etc. requiring efficient querying mechanisms [13, 14]. It is typical in medical research that multiple genetic features, their effects like diseases, and treatments to those diseases are studied together, often in a larger context such as medical history. One of the key challenge in cancer genomics – a cornerstone of precision medicine – is to discover gene-disease-drug associations which might be relevant for development new treatment methods. Such associations essentially correspond to paths in the semantic databases. It is exactly the paths that represent the associations and that need to be discovered, however SPARQL 1.1 does not provide adequate means for returning paths, only for testing reachability.

The lack of support of path enumeration and in SPARQL has long been recognized as an issue. There have been several surges of interest to the topic of implementing path queries in the context of SPARQL in the past decade which we briefly survey in Section 4.2. In particular, the European Semantic Web Conference in 2016 defined a challenge where the goal was exactly to find the “Top-K Shortest Path in Large Typed RDF Graphs” [18]. Only a handful of entries [10, 12, 20] were submitted where the winners approached the problem with tailored versions special purpose graph algorithms. What the short papers describing these approaches left out, was a systematic extension of SPARQL. It is surprising and unsatisfactory that still, even with numerous open source triple stores like Virtuoso and Jena, there is still no simple open source solution or extension library for top k-paths problems which one could use and extend.

In this paper, we aim to close exactly this gap: building on our prior work [8] we introduce an extension of SPARQL which allows us to find the top k shortest paths compliant with the property path expression. Using our syntax, the three most promising connections could be obtained with the following query:

Listing 2: Query using the :topk function

```
SELECT ?path WHERE{
  ?path ppath:topk (:me :alice 3 "foaf:knows+")}
```

Technically, our solution uses a built-in extension functionality of Jena ARQ and works out of the box with the Jena API¹ without a need to recompile the Jena code or modify its syntax.

In the remainder of this paper, after presenting the preliminaries (Section 2) we will present the syntax and semantics of the :topk function (section 3), and provide a simple but functionally complete evaluation strategy based on an efficient indexing with HDT and on the bidirectional breath-first search (Section 4) with the support of path restrictions via regular expressions. As we can show in our evaluation Section 4.1, our proposed solution of path computation on a HDT backend offers a very promising performance tackling graphs with tens of millions of triples. In particular, as we mention in a related work survey in Section 4.2, it outperforms

the approaches in [10, 12, 20]. Concluding remarks and a note on future work are offered in Section 5.

2 PRELIMINARIES

We assume a simplified RDF model representing graph data as a set of *subject-predicate-object* (spo) triples $\mathcal{I} \cup \mathcal{B} \times \mathcal{I} \times (\mathcal{I} \cup \mathcal{B} \cup \mathcal{L})$ where \mathcal{I} is a set of globally unique resource identifiers (IRIs), \mathcal{L} is the set of data values, or literals, and \mathcal{B} is the set of placeholders known as *blank nodes*. The triples form a labeled directed graph G . Specifically, each edge of G is a triple (s, p, o) where s is a subject or a *source node*, p is a predicate or an *edge label* and o is an object or a *target node*. We define a *path* in G as an ordered sequence of edges (e_1, \dots, e_n) such that (i) all edges in the path are *unique* i.e., $e_k \neq e_m$ for all integer $k, m \leq n$, and (ii) adjacent edges have a common incident node: that is, for every i the target node of e_i equals the source node of e_{i+1} if both edges are in a path. The source node of p is the source node of the first edge in it, and the target node of p is the target node t of the last edge in p , in which case p is called a *path from s to t* . If the source and the target node of a path coincide, it is called a *cycle*. According to our definition, paths can contain cycles: the same node can occur multiple times, but repeating edges are not allowed. Using standard graph terminology, our graph G is a *multigraph*, and every cycle in a path needs to be a *trail*, that is a cycle *without repeated edges*. The *length* of the path p is a number of edges in it. By $P_G(s, t)$ we denote the set of all paths from s to t in G , and by $\mathcal{P}_G^{asc}(s, t)$ we denote a sequence of all elements of $P_G(s, t)$ sorted in the order of non-decreasing lengths.

Our definition of path expressions is close to the SPARQL1.1 specification of property paths, up to inverse properties which we currently do not support in our implementation (but which could w.l.o.g. be considered as syntactic sugar).² Specifically, the following syntax is supported:

$$P := Q^* \mid Q^+ \mid Q^? \\ Q := a \mid ![a_1, \dots, a_k] \mid (P/P) \mid (P|P)$$

Here Q denotes an expression without occurrence restrictions, the unary quantifiers $*$, $+$ and $?$ respectively denote an unrestricted number of occurrences, at least a single occurrence and at most a single occurrence of a respective pattern Q . $a \in \mathcal{I}$ is an IRI representing a property, the set negation $![a_1, \dots, a_k]$, for $a_1, \dots, a_k \in \mathcal{I}$ is satisfies by any single property $b \in \mathcal{I} \setminus \{a_1, \dots, a_k\}$. Finally, (P/P) defines a sequence of path expressions and $(P|P)$ stipulates that only one of the expressions on the left and on the right of $|$ need to be satisfied. Both binary operators are associative, so we will omit parentheses in sequences of repeated binary operators of the same kind. The top k shortest paths problem is defined below:

Given an RDF graph G , $s \in \mathcal{I}$, $t \in \mathcal{I} \cup \mathcal{L}$, an integer k , and a regular path expression p .
Compute first k elements of $\mathcal{P}_G^{asc}(s, t)$ satisfying p .

For our computation, we will rely on a compressed index representation for RDF graphs called *HDT*: HDT[7] is a compact representation of RDF triples encoding verbose textual IRIs, literals and blank nodes as integers in an optimal way from the information

¹<https://jena.apache.org/documentation/query/library-propfunc.html>

²Note that inverse edges with specially marked inverse edge labels could be added to any graph by at maximum doubling the number of edges, thus not changing the overall complexity of graph processing.

theoretic point of view (i.e., assigning smallest values to most frequent items in the dataset). HDT supports the three-way indexing of triples, which is crucial for the performance of our algorithm.

3 SPARQL SYNTAX EXTENSION AND IMPLEMENTATION IN JENA

Our goal is to provide an implementation that can be embedded into the existing open source SPARQL engines, in particular Jena ARQ³ without a need of changing any legacy code. Although not part of any official specification, Jena SPARQL extension interfaces can be seen as a de facto standard which we make use of.

Our implementation of the basic, but robust solution for the k shortest path problem is based on bidirectional search: both the source and the target node of the paths need to be specified like in most routing tasks. The number of desired paths k defaults to 1, and the path pattern P defaults to the path pattern $(! : *)$:⁴ these arguments can either be omitted or should be bound to a constant of type integer and a string describing a path expression, respectively. The Jena ARQ framework allows SPARQL variables to occur at the input argument positions: our function requires those variables to also occur elsewhere in the query to ensure that at the point the topk function is called ARQ all its input parameters are bound (analogous to the notion of safety [19] in Datalog). Upon each call (for each binding of s and t , the topk function queries the RDF graph again and computes the shortest paths between s and t as explained in the next section. For each input tuple, there are up to k output values each representing a path. In our approach, we opted to encode the found paths as strings which can be then parsed by the calling applications to extract the properties and resources involved.

The type of Jena ARQ extension mechanism catering for all above desiderata is known as *property function*. Syntactically property functions use infix notation, appearing in the WHERE clause of SPARQL query as triples: the function is in the predicate position (predicates are often called properties, hence the name “property function”).

Both the values in the subject and in the object positions are passed to the function as arguments, whereby one of the two is meant to be the output and hence needs to contain an unbound variable. To pass multiple arguments, RDF lists need to be used. The predicate denoting functions can be distinguished by a dedicated namespace. The first option is to directly instruct ARQ which Java class to instantiate using a pseudo-url “java:(java.namespace.)”. The SPARQL function name needs to coincide with the name of the Java class implementing it in this case, which is not always convenient. The other way is to use a special registry of IRIs that resolve to property functions (such as `ppath:topk`) in our example. Such a registry is provided by ARQ. The downside of this approach is a slight increase of boilerplate code and, most importantly, the necessity to rebuild the calling Java program, which rules out this option for existing applications with dynamic queries like Jena Fuseki⁵. When the matching between the special predicate name and the Java function is established by ARQ, the function is called

for each tuple of constants binding the variables occurring in the triple that represent the property function call. The function `topk` is put into action in the small example in listing 2.

4 ALGORITHM

The core of our approach⁶ is the implementation of the topk function itself, which we solve with a relatively simple approach: our starting point is a bidirectional breath first search algorithm [8] which demonstrates good performance on HDT graphs in the ESWC 2016 challenge examples based on the DBpedia SPARQL Benchmark [17]: indeed as we can show, this approach outperforms any of the tailored algorithms submitted to the ESWC challenge.

Herein, we extend the algorithm from [8] with path pruning based on path expressions, provide an implementation which is easy to adapt to arbitrary graph models, and incorporates the path search in full SPARQL via the extension function mentioned in the previous section. The listing of the extended path search algorithm can be found below as algorithm 1.

The bidirectional breadth-first search (BFS) algorithm maintains the sets f_f and f_b of resources (RDF nodes) called *frontiers*: before the i -th iteration of the search procedure, f_f contains references to resources reachable from the source in exactly $\lfloor i/2 \rfloor$ steps, and f_b refers to resources reachable from the target node in exactly $\lfloor (i-1)/2 \rfloor$ steps. At each iteration, either the forward frontier f_f (odd i) or the backward frontier f_b (even i) is advanced. A resource α referenced by both frontiers before the iteration i belongs to a path of length $i-1$. Since BFS is used, all paths of the specified length are identified at the respective iteration of the algorithm. The finding of [8] is the way of maintaining the set of *paths* from the two terminal nodes to the respective frontiers using linked lists, so that if two paths have common prefix, this prefix is only represented once in the memory. Thus, the actual data items stored in frontiers are *traversal edges* (n, e, pr, γ) where n denotes the node, e is the incident edge via which this node has been reached, pr is the reference to the preceding traversal edge $(n_p, e_p, pr_p, \gamma_p)$ constructed at the previous advance step in the same direction, that is, on the one before previous iteration (the forward and the backward frontiers are advanced interchangeably). The meaning of γ is explained below.

To account for the property path pattern P in the process of search, we convert it into a nondeterministic finite automaton (NFA) using the library `dk.brics.automaton`[16] by Anders Møller. The implementation is based on character strings. Thus, in a pre-processing step (not shown in algorithm 1), we map each property mentioned in the path expression P to a unique character. Furthermore, a special character \perp is reserved to represent properties not used in P : such properties are not distinguished by P , therefore for the admissibility w.r.t. P , all such properties can be represented by one and the same symbol. The overall size of P is limited by the number of Unicode characters, which is perfectly sufficient in practice.

To cater for path checking also in the backward search, the second automaton based on the *inverse* of the path expression P is used: to invert P in our property path language it suffices to recursively reverse all sequences occurring in P : that is, replace every sequence

³<https://jena.apache.org/>

⁴We assume that the default namespace URI ‘:’ does not occur as a term in the dataset.

⁵https://jena.apache.org/documentation/serving_data/

⁶Available online at <https://bitbucket.org/vadim.savenkov/topk-pfn>

Algorithm 1 Bidirectional BFS with Pattern Enforcement via NFA

```

1: procedure BIDIRECTIONALBFS( $G, start, target, k, P$ )
2:    $sol \leftarrow \emptyset$  ▷ Solutions: shortest paths
3:    $A_f \leftarrow \text{Automaton}(P)$  ▷ RegExp  $P$  to NFA
4:    $A_b \leftarrow \text{Automaton}(\text{inverse}(P))$  ▷ Inverse of  $P$  to NFA
5:    $f_f \leftarrow (start, \text{null}, \text{null}, \gamma_{\text{init}}^{A_f})$  ▷ Forward frontier
6:    $f_b \leftarrow (target, \text{null}, \text{null}, \gamma_{\text{init}}^{A_b})$  ▷ Backward frontier
7:    $(fact, A_{act}) \leftarrow (f_f, A_f)$  ▷  $f_f$  is the active frontier
8:    $(f_{pass}, A_{pass}) \leftarrow (f_b, A_b)$ 
9:   while  $|sol| \leq k$  and not both  $f_f, f_b$  stable do
10:    if ADVANCE( $fact, A_{act}$ ) then
11:       $sol \leftarrow sol \cup \text{filter}(P, \text{JOIN}(f_f, f_b))$ 
12:    else
13:      Mark  $fact$  as stable.
14:    end if
15:    swap( $fact, A_{act}$ )  $\leftrightarrow$  ( $f_{pass}, A_{pass}$ )
16:  end while
17:  return  $sol$ 
18: end procedure

19: procedure ADVANCE( $f, A$ )
20:    $f' \leftarrow \emptyset$ 
21:    $\text{inc} = \begin{cases} \text{successor} & \text{if } f \text{ is the forward frontier} \\ \text{predecessor} & \text{otherwise} \end{cases}$ 
22:   for  $(n, e, pr, \gamma) \in f$  do
23:     for  $(e', n') \in \text{inc}(n)$  do
24:        $\gamma' \leftarrow \text{nextstate}(A, \gamma, e')$ 
25:       if  $\gamma' \neq \text{reject}$  then
26:          $f' \leftarrow f' \cup \{(n', e', (n, e, pr, \gamma), \gamma')\}$ 
27:       end if
28:     end for
29:   end for
30:   if  $f \neq \emptyset$  then
31:     Update the active frontier:  $f \leftarrow f'$ 
32:   else
33:     return fail
34:   end if
35: end procedure

36: function JOIN( $f_f, f_b$ )
37:    $res \leftarrow \emptyset$ 
38:   for  $(n, e_1, pr_1, \gamma_1) \in f_f, (n, e_2, pr_2, \gamma_2) \in f_b$  do
39:      $res \leftarrow res \cup \text{trace}(n, e_1, pr_1) \cdot \text{trace}(n, e_2, pr_2)$ 
40:   end for
41:   return  $res$ 
42: end function

```

(P_1/P_2) with (P_2/P_1) . Longer sequences $(P_1/\dots/P_k)$ (which we allow by virtue of associativity of $/$) are inverted as $(P_k/\dots/P_1)$. Two NFAs A_f and A_b are obtained respectively from the path expression P and its inverse P' . At the frontier advancement step, for a node n in a frontier tuple (n, e, pr, γ) , we only follow those incident edges e of n which are not rejected by the respective automaton A in its step γ (e is an outgoing edge for the forward frontier and incoming for the backward one).

	Triples	Subjects	Pred's	Objects	Shared
0.1DB	9264609	313036	13114	3482820	58535
1DB	46275619	1457983	21875	13751780	462478

Table 1: Datasets statistics

Start node	Target node	Property
dbr:Felipe_Massa	dbr:Red_Bull	dbp:firstWin
dbr:1952_Winter_Olympics	dbr:Elliot_Richardson	dbp:after
dbr:Karl_W._Hofmann	dbr:Elliot_Richardson	dbp:predecessor
dbr:Karl_K._Polk	dbr:Felix_Grundy	dbp:president

Table 2: Input parameters

4.1 Evaluation

We experimented with two datasets from the DBpedia SPARQL Benchmark [17] used in “Top-k Shortest Paths in large typed RDF Datasets Challenge”⁷ which was part of the 13th European Semantic Web Conference in 2016. Our hardware setup was a quad-core Intel i5 desktop machine with 8GB RAM. The used datasets correspond to the 10% sample and to the full benchmark dataset, which we respectively denote 0.1DB and 1DB. The data is freed from blank and untyped nodes. Table 1 lists the total number of triples, distinct subjects (IRIs), predicates, and objects, as well as the number of IRIs that occur both in the subject and the object position in the dataset. It is clear from the dataset statistics that the number of such shared objects is relatively small, within one promille of the number of triples.

Our experiment is based on the queries of the ESWC '16 challenge, which were four distinct pairs of start and target IRIs and two parameters, namely the value of k and an additional path restriction present in the half of the cases. All restrictions had the pattern $(\langle \text{property} \rangle / ! * | ! * / \langle \text{property} \rangle)$ thus stipulating that admissible paths either start or end with a specific property. All combinations of input parameters used in the challenge are given in Table 2.

Listing 3 presents the query that computes required paths for one of the tasks using our property function topk.

```

PREFIX : <http://dbpedia.org/property/>
PREFIX dbr: <http://dbpedia.org/resource/>
PREFIX ppf: <http://wu.ac.at/sparql/pathfn#>
SELECT ?path WHERE {
  ?path ppf:topk (dbr:Karl.W._Hofmann dbr:Elliot.Richardson
                 8088 "predecessor /!* | !*/predecessor" ) }

```

Listing 3: SPARQL query 10 k paths

We summarize the results of this experiment graphically in the following three figures. The first figure shows the dependency between the running time and the values of k used in different tasks. Note that not all tasks have the same values of k therefore the chart is not monotone, however one can see the trend of the running time increase with the growth of k . The two lines in Figure 1 show the average performance of the queries based on Table 2, for the tasks with and without path expressions. The dependency is not strictly monotone since not all queries are evaluated with the same values of k in the challenge. However, one can see that (i) the impact of path expressions on the performance in this particular

⁷cf. <https://bitbucket.org/ipapadakis/eswc2016-challenge/downloads/>

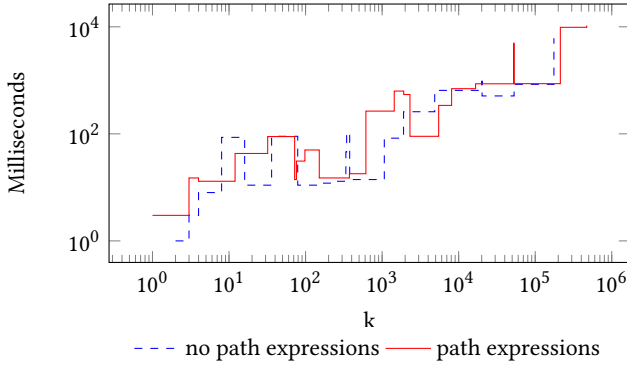


Figure 1: Performance of the ESWC'16 challenge queries

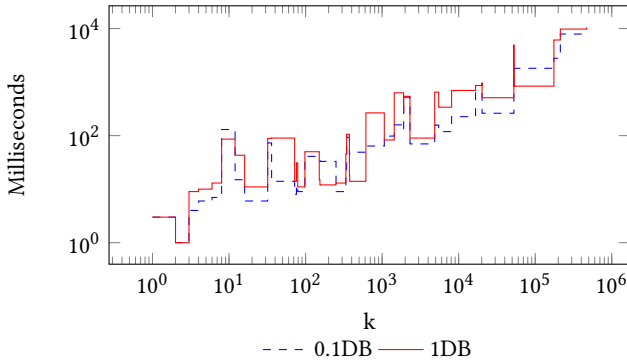


Figure 2: Performance of the ESWC'16 challenge queries for the 0.1DB and 1DB

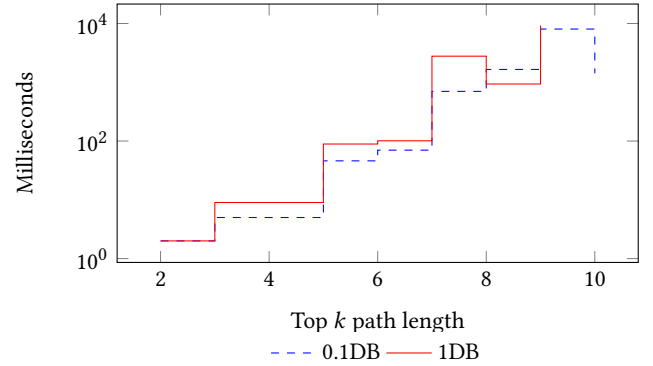
case is negligible (2) the dependency on k is linear (both axes in the figure are logarithmic).

Figure 2 shows the performance of exactly the same set of queries run against the 0.1DB and the full DBpedia Benchmark dataset 1DB. Noteworthy, an intuition of the same queries performing faster on smaller input is totally misleading for the top k paths queries. The reason is that the k th shortest path computed on sampled data tends to be longer than if computed on the full dataset, same nodes in which have higher degree. For instance, the longest path for the sample is of length 10, and of length 9 for the full case. For 10 out of 38 queries of the challenge, the maximal path length on the 0.1DB was exceeding the maximal path length on 1DB by 20 to 25%. As a consequence, the search for k may take longer and thus the performance is sometimes worse on 0.1DB as Figure 3 shows.

In all cases, and on the HDT backend, our algorithm was able to compute every single path in the maximum of 9 and 10 seconds respectively for the 0.1DB and 1DB. The median running time is 46 ms, the average for the 0.1DB is 652 ms and for 1DB 929 ms. Each task with k smaller than 100 took at most 112 ms to solve.

4.2 Related Work

Although path search is one of the most studied problems in Computer Science and also central in the Semantic Web area, the top k shortest path problem has not received sufficient attention in the

Figure 3: Performance of the ESWC'16 challenge queries by the top k path length for 0.1DB and 1DB

Semantic Web context so far. In fact, to the best of our knowledge the three ESWC'16 Challenge submissions [11], [12], [5] were the first to deal with the top k path computation specifically. The winner approach by Herling et al. [12] applied the Eppstein routing algorithm [6], which was designed for weighted graphs. In [5] the authors focus on decentralized computation and [11] developed an extension of the algebraic algorithm based on matrix multiplication and a special ρ -index structure. The primary benefit of our solution compared with the mentioned works is performance: due to the use of HDT-based indexing, for all reported queries our algorithm is at least the order of magnitude faster than any of the aforementioned solutions. The second benefit of our system is the possibility of using it with the standard systems out of the box. Having tested it with the HDT backend, we based our implementation on the standard Jena ARQ extension specification which makes it applicable to a broad range of systems supporting this API.

Beyond the scope of top k path queries, the literature on property path computation in the SPARQL context is broad. One of the earliest published accounts on addressing path queries was SPARQLer [15] and a comprehensive path query processor SPARQ2L [2]. Both approaches extend SPARQL with *path variables* (prepended by % or ?? instead of the usual single ?) instantiated by paths in queries such as `SELECT %path WHERE {<r> %path <s>}`. Additional possibilities of extracting individual resources from the path, filtering paths using path expressions and length restrictions (in the FILTER operator) and comparing paths, e.g. testing them for equality is supported. Neither of the two systems support top k path queries: to limit the number of retrieved results, one needs to restrict the path length in the filter condition. Ten years past the publication date, neither SPARQ2L nor SPARQLer system seem to be in use, freely available online for download or can be combined with the main open source SPARQL engines such as Jena ARQ or Virtuoso.

A path extension has been also reported for the efficient RDF3X engine [9]. With the syntax close to the previous two systems, RDF3X_path only finds a single shortest path, not an arbitrary k ones. The extension is tightly incorporated into the RDF3X code-base and cannot be used independently. One of the most comprehensive syntactical extensions of SPARQL has been undertaken by the CPSPARQL engine [1], where regular path expressions are

extended with constraints on resources (nodes) occurring within paths. Again, top k path queries are not supported, and although an implementation of the system is available, the focus of research is on the flexible and expressive language itself rather than on efficacy of query evaluation. No performance results on large graphs have been reported for CPSPARQL to the best of our knowledge.

5 CONCLUSIONS

We presented an efficient solution for the k shortest path problem in the context of SPARQL. Our function is based on the adaptation of the bidirectional breadth first search to top k paths computation [8], extending it with path expressions and embedding into Jena ARQ via the standard extension interface of property functions. On the indexed HDT backend, our implementation demonstrates very promising performance even without optimizations, which remain our main subject of future work. The source code of our implementation is openly available.

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