

¹Specification of regular constraints in SPARQL propert paths: <https://www.w3.org/TR/sparql11-property-paths/>. Access date: 07.07.2020.

problem nowadays, and new algorithms and solutions are being created [35, 46].

At the same time, utilization of more powerful languages, namely context-free languages, gain popularity in the last few years. *Context-Free Path Querying* problem (CFPQ) was introduced by Mihalis Yannakakis in 1990 in [47]. A number of different algorithms was proposed since that time, but recently, in [29] Jochem Kuijpers et al. show that state-of-the-art CFPQ algorithms are not performant enough to be used in practice. This fact motivates to find new algorithms for CFPQ.

One of the promising ways to achieve high-performance solutions for graph analysis problems is to reduce graph algorithms to linear algebra. This way, the description of basic linear algebra primitives, the GraphBLAS [26] API, was proposed. Solutions that use libraries that implement this API, such as SuiteSparse [15] and CombBLAS [9], show that reduction to linear algebra is a way to utilize high-performance parallel and distributed computations for graph analysis.

Rustam Azimov in [3] shows how to reduce CFPQ to matrix multiplication. Later, in [34] and [42], it was shown that utilization of appropriate libraries of linear algebra for Azimov's algorithm implementation allows one to get practical solution for CFPQ. But Azimov's algorithm requires transforming the input grammar to Chomsky Normal Form, which leads to the grammar size increase, thus worsen performance especially for regular queries and complex context-free queries.

To solve these problems, recently, an algorithm based on automata intersection was proposed [?]. This algorithm is based on linear algebra and does not require the input grammar transformation. In this work we improve it. First of all, we reduce it to operations over Boolean matrices, thus simplify its description and implementation. Also, we show that this algorithm is performant enough for regular queries, so it is a good candidate for integration with real-world query languages: we can use one algorithm to evaluate both regular and context-free queries.

Moreover, we show that this algorithm is a way to attack a long-standing problem of subcubic CFPQ. The best-known result for the general case is an $O(n^3/\log n)$ algorithm of Swarat Chaudhuri [12]. Also, there are solutions for partial cases. For example, there is a truly subcubic algorithm for 1-Dyck language proposed by Phillip Bradford [7]. But this solution cannot be generalized to arbitrary CFPQs. So, in our knowledge, there is no truly subcubic general algorithm for CFPQs. In this work we show that incremental transitive closure is a bottleneck on the way to get subcubic time complexity for CFPQ.

To summarize, we make the following contributions in this paper.

- (1) We rethink and improve tensor-product-based algorithm for CFPQ. First of all, we reduce this algorithm to operations over Boolean matrices. All paths semantics. Previous matrix-based solution only single path. For both regular and context-free path queries. Correctness and time complexity.
- (2) We demonstrate interconnection between CFPQ and incremental transitive closure. Conjecture on sublinear incremental transitive closure and subcubic CFPQ. We show that incremental transitive closure is a bottleneck on the way to get subcubic CFPQ algorithm.
- (3) By using existing results we show how to get slightly subcubic algorithm for general case, and subcubic combinatorial algorithm for partial cases. This criterion is output-sensitive, so it is not practical, but open a theoretical way to find more subclass with subcubic complexity.
- (4) We implement the described algorithm and evaluate it on real-world data. RPQ, CFPQ. Results show that !!!

2 PRELIMINARIES

In this section we introduce basic notation and definitions from graph theory and formal language theory which are used in our work.

2.1 Language-Constrained Path Querying Problem

We use a directed edge-labeled graph as a data model. To introduce the *Language-Constraint Path Querying Problem* [?] over directed edge-labeled graphs we should give both language and grammar definitions.

Definition 2.1. The edge-labeled directed graph $\mathcal{G} = \langle V, E, L \rangle$, where:

- V is a finite set of vertices
- $E \in V \times L \times V$ is a finite set of edges
- L is a finite set of edge labels

Since V has finite size, one can always introduce bijection between V and $Q = \{0, \dots, |V| - 1\}$, thus in our work we guess that $V = \{0, \dots, |V| - 1\}$.

The example of a graph which we use in further examples is presented in Figure 1.

Definition 2.2. Adjacency matrix for a edge-labeled directed graph $\mathcal{G} = \langle V, E, L \rangle$ is a matrix M , that:

- M has size $|V| \times |V|$
- $M[i, j] = \{l \mid \mid e = (i, l, j) \in E\}$

Adjacency matrix M_2 of the graph \mathcal{G} is



Figure 1: The example of input graph \mathcal{G}

$$M_2 = \begin{pmatrix} \cdot & \{a\} & \cdot & \cdot \\ \cdot & \cdot & \{a\} & \cdot \\ \{a\} & \cdot & \cdot & \{b\} \\ \cdot & \cdot & \{b\} & \cdot \end{pmatrix}.$$

Definition 2.3. Boolean matrices decomposition, or Boolean adjacency matrix, for a edge-labeled directed graph $\mathcal{G} = \langle V, E, L \rangle$ with adjacency matrix M is a set of matrices $\mathcal{M} = \{M^l \mid l \in L, M^l[i, j] = 1 \iff l \in M[i, j]\}$.

In our work we use decomposition of the adjacency matrix to a set of Boolean matrices. As an example, matrix M_2 can be represented as a set of two Boolean matrices M_2^a and M_2^b as presented in Figure 2.

$$M_2^a = \begin{pmatrix} \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, M_2^b = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & 1 & \cdot \end{pmatrix} \quad (1)$$

Figure 2: The representation of the matrix M_2 as a set of Boolean matrices

In this way we reduce operations which are necessary for our algorithm from operations over custom semiring (over edge labels) to operations over a Boolean semiring.

In this work we also use the following notation $\mathcal{M}(\mathcal{G})$ and $\mathcal{G}(\mathcal{M})$ to describe the Boolean decomposition matrices for some graph and the graph formed by its adjacency Boolean matrices correspondingly.

Also, we should define the path in the graph and the word formed by the path.

Definition 2.4. Path π in the graph $\mathcal{G} = \langle V, E, L \rangle$ is a sequence e_0, e_1, \dots, e_{n-1} , where $e_i = (v_i, l_i, u_i) \in E$ and for any e_i, e_{i+1} $u_i = v_{i+1}$. We denote path from v to u as $v\pi u$.

Definition 2.5. The word formed by a path

$$\pi = (v_0, l_0, v_1), (v_1, l_1, v_2), \dots, (v_{n-1}, l_{n-1}, v_n)$$

is a concatenation of labels along the path: $\omega(\pi) = l_0 l_1 \dots l_{n-1}$.

The next part is a definitions from the formal language theory.

Definition 2.6. A language \mathcal{L} over a finite alphabet Σ is a subset of all possible sequences formed by symbols from the alphabet: $\mathcal{L}_\Sigma = \{\omega \mid \omega \in \Sigma^*\}$.

Now we are ready to introduce CFPQ problem for the given graph $\mathcal{G} = \langle V, E, L \rangle$ and the given language \mathcal{L} with reachability and all paths semantics.

Definition 2.7. To evaluate context-free path query with reachability semantics is to construct a set of pairs of vertices (v_i, v_j) such that there exists a path $v_i \pi v_j$ in \mathcal{G} which forms the word from the given language:

$$R = \{(v_i, v_j) \mid \exists \pi : v_i \pi v_j, \omega(\pi) \in \mathcal{L}\}$$

Definition 2.8. To evaluate context-free path query with all paths semantics is to construct a set of paths π in \mathcal{G} which form the word from the given language:

$$\Pi = \{\pi \mid \omega(\pi) \in \mathcal{L}\}$$

Note that Π can be infinite, thus in practice, we should provide a way of enumerating such paths with reasonable complexity, instead of explicit construction of the Π .

2.2 Regular Path Queries and Finite State Machine

The first case of language-constrained path querying is *Regular Path Querying* (RPQ): the language L is a regular language. This case is widely spread in practice [?].

Usual way to specify regular languages is *regular expressions*. We use the following definition of regular expressions.

Definition 2.9. Regular expression (and regular language) over alphabet Σ can be inductively defined as follows.

- \emptyset (empty language) is regular expression
- ε (empty string) is regular expression
- $a_i \in \Sigma$ is regular expression
- if R_1 and R_2 are regular expressions, then $R_1 \mid R_2$ (alternation), $R_1 \cdot R_2$ (concatenation), R_1^* (Kleene star) are also regular expressions.

For example, one can specify regular expression $R_1 = ab^*$ to find paths in the graph \mathcal{G} (fig. 1). Expected result is set of paths which start with a -labeled edge and contain zero or more b -labeled edges after that.

In this work we use the notion of *Finite-State Machine* (FSM) or *Finite-State Automaton* (FSA) for RPQs.

Definition 2.10. Deterministic Finite-State Machine T is a tuple $\langle \Sigma, Q, Q_s, Q_f, \delta \rangle$ where

- Σ is an input alphabet,
- Q is a finite set of states,
- $Q_s \subseteq Q$ is a set of start (or initial) states,

- $Q_f \subseteq Q$ is a set of final states,
- $\delta : Q \times \Sigma \rightarrow Q$ is a transition function.

It is well known, that every regular expression can be converted to deterministic FSM without ε -transitions. To do it one can use [23]. In our work we use FSM as a representation of RPQ. FSM can be naturally represented by a directed edge-labeled graph: $V = Q$, $L = \Sigma$, $E = \{(q_i, l, q_j) \mid \delta(q_i, l) = q_j\}$, where some vertices have special markers to specify start and final states. Example of graph-style representation of FSM T_1 for the regular expression R_1 is presented in Figure 3.

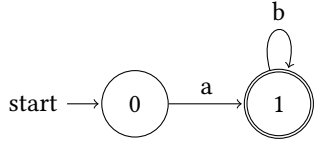


Figure 3: The example of graph representation of FSM for the regular expression ab^*

As a result, FSM also can be represented as a set of Boolean adjacency matrices M with additional information about start and final vertices. Such representation of T_1 is presented in Figure 4.

$$M^a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad M^b = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Figure 4: The representation of the FSM T_1 as a set of Boolean matrices

Note, that the edge-labeled graph is an FSM: edges are transitions, all vertices should be both start and final at the same time. Thus RPQ evaluation is an intersection of two FSMs, and the result also can be represented as FSM, because regular languages are closed under intersection.

2.3 Context-Free Path Querying and Recursive State Machines

An even more general case, than RPQ, is a *Context-Free Path Querying Problem (CFPQ)*, where one can use context-free languages as constraints. These constraints are more expressive than the regular ones, for example, one can express classical same-generation query using context-free language, but not a regular one.

Definition 2.11. Context-free grammar $G = \langle \Sigma, N, S, P \rangle$ where Σ is a finite set of terminals (or terminal alphabet), N is a finite set of nonterminals (or nonterminal alphabet), $S \in N$ is a start nonterminal, and P is a finite set of productions (grammar rules) of form $N_i \rightarrow \alpha$ where $N_i \in N$, $\alpha \in (\Sigma \cup N)^*$.

Definition 2.12. The sequence $\omega_2 \in (\Sigma \cup N)^*$ is derivable from $\omega_1 \in (\Sigma \cup N)^*$ in one derivation step, or $\omega_1 \rightarrow \omega_2$, in the grammar $G = \langle \Sigma, N, S, P \rangle$ iff $\omega_1 = \alpha N_i \beta$, $\omega_2 = \alpha \gamma \beta$, and $N_i \rightarrow \gamma \in P$.

Definition 2.13. Context-free grammar $G = \langle \Sigma, N, S, P \rangle$ specifies a *context-free language*: $\mathcal{L}(G) = \{\omega \mid S \xrightarrow{*} \omega\}$, where $(\xrightarrow{*})$ denotes zero or more derivation steps (\rightarrow) .

Thus, one can use the grammar $G_1 = \langle \{a, b\}, \{S\}, S, \{S \rightarrow a b; S \rightarrow a S b\} \rangle$ to find paths which form words in the language $\mathcal{L}(G_1) = \{a^n b^n \mid n > 0\}$ in the graph \mathcal{G} (fig. 1).

Regular expressions can be transformed to a FSM, and a context free grammar can be transformed to *Recursive State Machine* (RSM) (also known as recursive networks [?], recursive automata [?], !!!.) in the similar way. In our work we use the following definition of RSM.

Definition 2.14. A recursive state machine R over a finite alphabet Σ is defined as a tuple of elements $(M, m, \{C_i\}_{i \in M})$, where:

- M is a finite set of labels of boxes.
- $m \in M$ is an initial box label.
- Set of *component state machines* or *boxes*, where $C_i = (\Sigma \cup M, Q_i, q_i^0, F_i, \delta_i)$:
 - $\Sigma \cup M$ is a set of symbols, $\Sigma \cap M = \emptyset$
 - Q_i is a finite set of states, where $Q_i \cap Q_j = \emptyset, \forall i \neq j$
 - q_i^0 is an initial state for C_i
 - F_i is a set of final states for C_i , where $F_i \subseteq Q_i$
 - $\delta_i : Q_i \times (\Sigma \cup M) \rightarrow Q_i$ is a transition function

RSM behaves as a set of finite state machines (or FSM). Each FSM is called a *box* or a *component state machine* [1]. A box works almost the same way as a classical FSM, but it also handles additional *recursive calls* and employs an implicit *call stack* to *call* one component from another and then return execution flow back.

The execution of an RSM could be defined as a sequence of the configuration transitions, which are done on input symbols reading. The pair (q_i, S) , where q_i is current state for box C_i and S is stack of *return states*, describes execution configurations.

The RSM execution starts from configuration $(q_m^0, \langle \rangle)$. The following list of rules defines the machine transition from configuration (q_i, S) to (q', S') on some input symbol a from input sequence, which is read as usual for FSA:

- $(q_i^k, S) \rightsquigarrow (\delta_i(q_i^k, a), S)$
- $(q_i^k, S) \rightsquigarrow (q_j^0, \delta_i(q_i^k, j) \circ S)$
- $(q_j^k, q_i^t \circ S) \rightsquigarrow (q_i^t, S)$, where $q_j^k \in F_j$

Some input sequence of the symbols $a_1 \dots a_n$, which forms some input word, is accepted, if machine reaches configuration $(q, \langle \rangle)$, where $q \in F_m$. It is also worth noting that the RSM makes nondeterministic transitions, without reading

the input character when it *calls* some component or makes a *return*.

According to [1], recursive state machines are equivalent to pushdown systems. Since pushdown systems are capable of accepting context-free languages [23], it is clear that RSMs are equivalent to context-free languages. Thus RSMs suit to encode query grammars. Any CFG can be easily converted to an RSM with one box per nonterminal. The box which corresponds to a nonterminal A is constructed using the right-hand side of each rule for A .

An example of such RSM R constructed for the grammar G with rules $S \rightarrow aSb \mid ab$ is provided in Figure 5. For a given example of the grammar and the RSM consider the following sequence of the machine configuration transitions, in case, where one want to determine, if input word $aabb$ belongs to the language $L(G)$. The RSM execution starts from configuration $(q_S^0, \langle \rangle)$, reads symbols a and goes to $(q_S^1, \langle \rangle)$. Then, in the nondeterministic manner it tries to read b but fails, and in the same time tries to derive S and goes to configuration $(q_S^0, \langle q_S^2 \rangle)$, where q_S^2 is *return* state. Then machine reads a and goes to $(q_S^1, \langle q_S^2 \rangle)$. In this case, in the nondeterministic choice it fails to derive S , but successfully reads b and goes to configuration $(q_S^3, \langle q_S^2 \rangle)$. Since q_S^3 is final state for the box S , the RSM tries to make *return* and goes to $(q_S^2, \langle \rangle)$. Then it reads b and transits to $(q_S^3, \langle \rangle)$. Since $q_S^3 \in F_S$ and the *return* stack is empty, the machine accepts the input sequence $aabb$.

Since R is a set of FSMs, it is useful to represent R as an adjacency matrix for the graph where vertices are states from $\bigcup_{i \in M} Q_i$ and edges are transitions between q_i^a and q_i^b with label $l \in \Sigma \cup M$, if $\delta_i(q_i^a, l) = q_i^b$. An example of such adjacency matrix M_R for the machine R is provided in section ??.



Figure 5: The recursive state machine R for grammar G

Similarly to a FSM, an RSM can be representaed as a graph and, hence, as a set of Boolean adjacency matrices. For our example, M_1 is:

$$M_1 = \begin{pmatrix} \cdot & \cdot & \{a\} & \cdot \\ \cdot & \cdot & \{S\} & \{b\} \\ \cdot & \cdot & \cdot & \{b\} \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Matrix M_1 can be represented as a set of Boolean matrices as follows:

$$M_1^S = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, M_1^a = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, M_1^b = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Similarly to an RPQ, a CFPQ is the intersection of the given context-free language and a FSM specified by the given graph. As far as every context-free language is closed under intersection with regular languages, such intersection can be represented as an RSM. Also, one can look at the RSM as a FSM over $\Sigma \cup N$. In this work we use this point of view to propose unified algorithm for evaluation both regular and context-free path queries with zero overhead for regular ones.

2.4 Graph Kronecker Product and Machines Intersection

First of all, we introduce classical Kronecker product definition, describe graph Kronecker product and its relation to Boolean matrices algebra, RSM and FSM intersection.

Definition 2.15. Given two matrices A and B of sizes $m_1 \times n_1$ and $m_2 \times n_2$ respectively, with element-wise product operation \cdot . The Kronecker product of these two matrices is a new matrix $C = A \otimes B$, where:

- C has size $m_1 * m_2 \times n_1 * n_2$
- $C[u * m_1 + v, n_1 * p + q] = A[u, p] \cdot B[v, q]$

It is worth mention, that the Kronecker product produces blocked matrix C , with total number of the blocks $m_1 * n_1$, where each block has size $m_2 * n_2$ and is defined as $A[i, j] \cdot B$ (scalar to matrix).

Definition 2.16. Given two edge-labeled directed graphs $\mathcal{G}_1 = \langle V_1, E_1, L_1 \rangle$ and $\mathcal{G}_2 = \langle V_2, E_2, L_2 \rangle$ the Kronecker product of these two graphs is a edge-labeled directed graph $\mathcal{G} = \mathcal{G}_1 \otimes \mathcal{G}_2$, where $\mathcal{G} = \langle V, E, L \rangle$:

- $V = V_1 \times V_2$
- $E = \{((u, v), l, (p, q)) \mid (u, l, p) \in E_1 \wedge (v, l, q) \in E_2\}$
- $L = L_1 \cap L_2$

The Kronecker product for graphs produces a new graph with a property, that if some path $(u, v)\pi(p, q)$ exists in the result graph then paths $u\pi_1 p$ and $v\pi_2 q$ exist in the input graphs, and $\omega(\pi) = \omega(\pi_1) = \omega(\pi_2)$. These paths π_1 and π_2 could be easily found from π by its definition.

The Kronecker product for directed graphs can be easily described as the Kronecker product of the corresponding adjacency matrices of graphs, what gives us the following definition:

Definition 2.17. Given two adjacency matrices M_1 and M_2 of sizes $m_1 \times n_1$ and $m_2 \times n_2$ respectively, for some directed

graphs \mathcal{G}_1 and \mathcal{G}_2 . The Kronecker product of these two adjacency matrices is the adjacency matrix M of a some graph \mathcal{G} , where:

- M has size $m_1 * m_2 \times n_1 * n_2$
- $M[u * m_1 + v, n_1 * p + q] = M_1[u, p] \cap M_2[v, q]$

By the definition, the Kronecker product for adjacency matrices gives an adjacency matrix with the same set of edges as in the resulting graph in the Def. 2.16. Thus, $M(\mathcal{G}) = M(\mathcal{G}_1) \otimes M(\mathcal{G}_2)$, where $\mathcal{G} = \mathcal{G}_1 \otimes \mathcal{G}_2$.

Definition 2.18. Given two FSMs $T_1 = \langle \Sigma, Q^1, Q_S^1, S_F^1, \delta^1 \rangle$ and $T_2 = \langle \Sigma, Q^2, Q_S^2, S_F^2, \delta^2 \rangle$. The intersection of this two machines is a new FSM $T = \langle \Sigma, Q, Q_S, S_F, \delta \rangle$, where:

- $Q = Q^1 \times Q^2$
- $Q_S = Q_S^1 \times Q_S^2$
- $Q_F = Q_F^1 \times Q_F^2$
- $\delta : Q \times \Sigma \rightarrow Q$, $\delta(\langle q_1, q_2 \rangle, s) = \langle q'_1, q'_2 \rangle$,
if $\delta(q_1, s) = q'_1$ and $\delta(q_2, s) = q'_2$

According to [23], the above definition of the FSM intersection allows to construct the new machine with the following property: $L(T) = L(T_1) \cap L(T_2)$.

The most computationally expensive part of such procedure is the δ function construction for the new machine T . Using adjacency matrices decomposition for FSMs we can reduce the intersection to the Kronecker product of such matrices over Boolean semiring at some extent, since the transition function δ of the machine T in matrix form is exactly the same as the product result. More precisely:

Definition 2.19. Given two adjacency matrices \mathcal{M}_1 and \mathcal{M}_2 over Boolean semiring. The Kronecker product of these matrices is a new matrix $\mathcal{M} = \mathcal{M}_1 \otimes \mathcal{M}_2$, defined as follows:

- $\mathcal{M} = \{\mathcal{M}_1^a \otimes \mathcal{M}_2^a \mid a \in \Sigma\}$
- The element-wise operation is *and* over Boolean values

Applying the Kronecker product theory for both the FSM and the edge-labeled directed graph, we can intersect this objects as shown in Def. 2.19, since the graph could be interpreted as an FSM with transitions matrix represented as the Boolean adjacency matrix.

In this work we show how to express RSM and FSM intersection in terms of Kronecker product and transitive closure over Boolean semiring.

3 CONTEXT-FREE PATH QUERYING BY KRONECKER PRODUCT

In this section, we introduce the algorithm for CFPQ which is based on Kronecker product of Boolean matrices. The algorithm provides the ability to solve all-pairs CFPQ in all-path semantics (according to Hellings [22]) and consists of the two following parts.

- (1) Index creation. In the first step, the algorithm computes an index which contains information which is necessary to restore paths for specified pairs of vertices. This index can be used to solve the reachability problem without paths extraction. Note that this index is finite even if the set of paths is infinite.
- (2) Paths extraction. All paths for the given pair of vertices can be enumerated by using the index computed at the previous step. As far as the set of paths can be infinite, all paths cannot be enumerated explicitly, and advanced techniques such as lazy evaluation are required for implementation. Anyway, a single path can be always extracted by using standard techniques.

We describe both these steps, prove correctness, and provide time complexity estimations. For the first step we firstly introduce naïve algorithm. After that we show how to achieve cubic time complexity by using dynamic transitive closure algorithm and demonstrate that this technique allow us to get truly subcubic CFPQ algorithm for planar graphs.

After that we provide step-by-step example of query evaluation by using the proposed algorithm.

3.1 Index Creation Algorithm

The *index creation* algorithm outputs the final adjacency matrix \mathcal{M}_2 for the input graph with all vertices pairs, which are reachable through some nonterminal in the input grammar G , and the index matrix C_3 , which allows to extract paths in the *path extraction* algorithm.

The algorithm is based on the generalization of the FSM intersection for an RSM, and the edge-labeled directed input graph. Since the RSM is composed as set of FSMs, it could be easily presented as adjacency matrix for some graph over labels set $\Sigma \cup S$. As shown in the Def. 2.19 we can apply Kronecker product from Boolean matrices to *intersect* the RSM and the input graph to some extent. But the RSM contains the nonterminal symbols from N with additional *recursive calls* logic, what requires *transitive closure* step for such symbols extraction.

Applying the Kronecker product and transitive closure theory together, we get the idea of the algorithm: iterative Kronecker product evaluation for the RSM and the input graph, followed by transitive closure, nonterminal extraction and the update of the graph adjacency matrix.

3.1.1 Boolean Matrices Based Version. Listing 1 shows main steps of the algorithm. The algorithm accepts context-free grammar $G = (\Sigma, N, P)$ and graph $\mathcal{G} = (V, E, L)$ as an input. An RSM R is created from the grammar G . Note, that R must have no ε -transitions. \mathcal{M}_1 and \mathcal{M}_2 are the Boolean adjacency matrices for the machine R and the graph \mathcal{G} correspondingly.

Then for each vertex i of the graph \mathcal{G} , the algorithm adds loops with non-terminals, which allows deriving ε -word.

Here the following rule is implied: each vertex of the graph is reachable by itself through an ε -transition. Since the machine R does not have any ε -transitions, the ε -word could be derived only if a state s in the box B of the R is both initial and final. This data is queried by the *getNonterminals* function for each state s .

The algorithm terminates when the matrix M_2 stops changing. Kronecker product of matrices M_1 and M_2 is evaluated for each iteration. The result is stored in M_3 as a Boolean matrix. Since we are interested only in the reachability of some vertices, there is no need to store a separate Boolean matrix for each label from $\Sigma \cup N$. Therefore, we can collapse it into one Boolean matrix M'_3 , what is done in the next step. These Boolean matrix could be interpreted as an adjacency matrix for some directed graph without labels with the same set of the vertices, as in the graph formed by M_3 . From that point of view the matrix M'_3 has the following property from its definition: if some vertices connected by some path in the graph $\mathcal{G}(M'_3)$ then these vertices are connected by one or many paths in the graph $\mathcal{G}(M_3)$.

For the given M'_3 a C_3 transitive closure matrix is evaluated by the corresponding function call. Then the algorithm iterates over cells of the C_3 . For the pair of indices (i, j) , it computes s and f – the initial and final states in the recursive automata R which relate to the concrete $C_3[i, j]$ of the closure matrix. If the given s and f belong to the same box B of R , $s = q_B^0$, and $f \in F_B$, then *getNonterminals* returns the respective nonterminal. Then for each such nonterminal the respective matrix of the graph adjacency matrix M_2 is updated and a new edge as a Boolean value in the appropriate cell is added.

The functions *getStates* and *getCoordinates* (see Listing 2) are used to map indices between Kronecker product arguments and the result matrix. The Implementation appeals to the blocked structure of the matrix C_3 , where each block corresponds to some automata and graph edge.

The algorithm returns the computed path extraction index C_3 and the updated matrix M_2 , which contains the initial graph \mathcal{G} data as well as data for nonterminals from N . If a cell $M_2^S[i, j]$ for any valid indices i and j and $S \in N$ contains $\{1\}$, then vertex j is reachable from vertex i in grammar G for nonterminal S .

3.1.2 Index creation for RPQ. In case of the RPQ, the main **while** loop takes only one iteration to actually append data. Since the input query is provided in form of the regex, one can construct the corresponding RSM, which consists of the single *component state machine*. This CSM is built from the regex and labeled as the S for example, which has no *recursive calls*. The adjacency matrix of the machine is build over Σ only. Therefore, calculating the Kronecker product,

all relevant information is taken into account at the first iteration of the loop.

Listing 1 Kronecker product based CFPQ

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1: function CONTEXTFREEPATHQUERYING( $G, \mathcal{G}$ )
2:    $R \leftarrow$  Recursive automata for  $G$ 
3:    $M_1 \leftarrow$  Boolean adjacency matrix for  $R$ 
4:    $M_2 \leftarrow$  Boolean adjacency matrix for  $\mathcal{G}$ 
5:    $C_3 \leftarrow$  The empty matrix
6:   for  $s \in 0..dim(M_1) - 1$  do
7:     for  $S \in getNonterminals(R, s, s)$  do
8:       for  $i \in 0..dim(M_2) - 1$  do
9:          $M_2^S[i, i] \leftarrow \{1\}$ 
10:  while Matrix  $M_2$  is changing do
11:     $M_3 \leftarrow M_1 \otimes M_2$  ▷ Evaluate Kronecker product
12:     $M'_3 \leftarrow \bigvee_{M_3^a \in M_3} M_3^a$  ▷ Collapse to Boolean matrix
13:     $C_3 \leftarrow transitiveClosure(M'_3)$ 
14:     $n \leftarrow dim(M_3)$  ▷ Matrix  $M_3$  size =  $n \times n$ 
15:    for  $(i, j) \in [0..n - 1] \times [0..n - 1]$  do
16:      if  $C_3[i, j]$  then
17:         $s, f \leftarrow getStates(C_3, i, j)$ 
18:         $x, y \leftarrow getCoordinates(C_3, i, j)$ 
19:        for  $S \in getNonterminals(R, s, f)$  do
20:           $M_2^S[x, y] \leftarrow \{1\}$ 
21:  return  $M_2, C_3$ 

```

Listing 2 Help functions for Kronecker product based CFPQ

```

1: function GETSTATES( $C, i, j$ )
2:    $r \leftarrow dim(M_1)$  ▷  $mathcal{M}_1$  is Boolean adjacency matrix for  $R$ 
3:   return  $\lfloor i/r \rfloor, \lfloor j/r \rfloor$ 
4: function GETCOORDINATES( $C, i, j$ )
5:    $n \leftarrow dim(M_2)$  ▷  $M_2$  is Boolean adjacency matrix for  $\mathcal{G}$ 
6:   return  $i \bmod n, j \bmod n$ 

```

LEMMA 3.1. *Let $\mathcal{G} = (V, E, L)$ be a graph and $G = \langle \Sigma, N, S, P \rangle$ be a grammar. Let $M_{2,(k)}$ be an adjacency matrix M_2 after the execution of some iteration $k \geq 0$ of the algorithm in Listing 1. Then for any valid indices i, j and for each nonterminal $A \in N$ such that cell $M_{2,(k)}^A[i, j]$ contains $\{1\}$, the following statement holds: in the graph $\mathcal{G} \exists i\pi j : A \xrightarrow{*} l(\pi)$.*

PROOF. (Proof by induction)

Basis: For $k = 0$ and the statement of the lemma holds, since $M_{2,(0)} = M_2$, where M_2 is adjacency matrix of the graph \mathcal{G} . The nonterminals, which allow to derive ε -word, are also added at algorithm preprocessing step, since each vertex of the graph is reachable by itself through an ε -transition.

Inductive step: Assume that the statement of the lemma holds for any $k \leq (p - 1)$ and show that it also holds for $k = p$, where $p \geq 1$.

For the algorithm iteration p the Kronecker product M_3, M'_3 and transitive closure C_3 are evaluated as described in the

algorithm. By the properties of this operations, some edge $e = ((s, i), (f, j))$ exists in the directed graph, represented by adjacency matrix C_3 , if and only if $\exists s\pi'f$ in the RSM graph, represented by matrix \mathcal{M}_1 , and $\exists i\pi j$ in graph, represented by $\mathcal{M}_{2,(p-1)}$. Concatenated symbols along the path π' form some derivation string v , composed from terminals and non-terminals, where $v \xrightarrow{*} l(\pi)$ by the inductive assumption.

The new $\{1\}$ will be added to the cell $M_{2,(k)}^A[i, j]$ only if s and f are initial and final states of some box of the RSM corresponding to the non-terminal A . In this case, the grammar G has the derivation rule $A \rightarrow v$, and by the inductive assumption $v \xrightarrow{*} l(\pi)$. Therefore, $A \xrightarrow{*} l(\pi)$ and this completes the proof of the lemma. \square

LEMMA 3.2. *Let $\mathcal{G} = (V, E, L)$ be a graph and $G = \langle \Sigma, N, S, P \rangle$ be a grammar. Let $\mathcal{M}_{2,(k)}$ be an adjacency matrix \mathcal{M}_2 after the execution of some iteration $k \geq 0$ of the algorithm in Listing 1. For any path $i\pi j$ in the graph \mathcal{G} with word $l = l(\pi)$ if exists the derivation tree of l from the nonterminal A of the grammar G with the height $h \leq k + 1$, then $M_{2,(k)}^A[i, j]$ contains $\{1\}$.*

PROOF. (Proof by induction)

Basis: Show that statement of the lemma holds for the $k = 0$. Matrix $\mathcal{M}_{2,(0)} = \mathcal{M}_2$ and edges of the graph \mathcal{G} contains only labels from L . Since the derivation tree of height $h = k + 1 = 1$ contains only one non-terminal A as a root and only symbols from $\Sigma \cup \varepsilon$ as leaves, for all paths, which form a word with derivation tree of the height $h = 1$, the corresponding nonterminals will be added to the $M_{2,(0)}^A[i, j]$ via preprocessing step. Thus, the lemma statement holds for the $k = 1$.

Inductive step: Assume that the statement of the lemma hold for any $k \leq (p - 1)$ and show that it also holds for $k = p$, where $p \geq 2$.

For the algorithm iteration p the Kronecker product $\mathcal{M}_3, \mathcal{M}'_3$ and transitive closure C_3 are evaluated as described in the algorithm. By the properties of this operations, some edge $e = ((s, i), (f, j))$ exists in the directed graph, represented by adjacency matrix C_3 , if and only if $\exists s\pi'f$ in the RSM graph, represented by matrix \mathcal{M}_1 , and $\exists i\pi j$ in graph, represented by $\mathcal{M}_{2,(p-1)}$.

For any path $i\pi j$, such that exist derivation tree of height $h < p + 1$ for the word $l(\pi)$ with root non-terminal A , the cell $M_{2,(p)}^A[i, j]$ contains $\{1\}$ by inductive assumption.

Suppose, that exists derivation tree T of height $h = p + 1$ with the root non-terminal A for the path $i\pi j$. The tree T is formed as $A \rightarrow a_1..a_d, d \geq 1$ where $\forall x \in [1..d] a_x$ is sub-tree of height $h_x \leq p$ for the sub-path $i_x\pi_xj_x$. By inductive hypothesis, there exists path π_x for each derivation sub-tree, such that $i = i_1\pi_1i_2..i_d\pi_dj_d = j$ and concatenation of these

paths forms $i\pi j$, and the root nonterminals of this sub-trees are included in the matrix $\mathcal{M}_{2,(p-1)}$.

Therefore, vertices $i_x \forall x \in [1..d]$ form path in the graph, represented by matrix $\mathcal{M}_{2,(p-1)}$, with complete set of labels. Thus, new $\{1\}$ will be added to the cell $M_{2,(p)}^A[i, j]$ corresponding to the vertices i and j and nonterminal A . This completes the proof of the lemma. \square

THEOREM 3.3. *Let $\mathcal{G} = (V, E, L)$ be a graph and $G = \langle \Sigma, N, S, P \rangle$ be a grammar. Let \mathcal{M}_2 be a result adjacency matrix after the execution of the algorithm in Listing 1. Then for any valid indices i, j and for each nonterminal $A \in N$ the following statement holds: the cell $M_{2,(k)}^A[i, j]$ contains $\{1\}$, if and only if there is a path $i\pi j$ in the graph \mathcal{G} such that $A \xrightarrow{*} l(\pi)$.*

PROOF. This theorem is a consequence of the Lemma 3.1 and Lemma 3.2. \square

THEOREM 3.4. *Let $\mathcal{G} = (V, E, L)$ be a graph and $G = \langle \Sigma, N, S, P \rangle$ be a grammar. The algorithm in Listing 1 terminates in finite number of steps.*

PROOF. The main *while-loop* in the algorithm is executed while graph adjacency matrix \mathcal{M}_2 is changing. Since the algorithm only adds the edges with non-terminals from N , the maximum required number of iterations is $|N| \times |V| \times |V|$, where each component has finite size. This completes the proof of the theorem. \square

3.1.3 Application of Dynamic Transitive Closure. In this subsection we show how to reduce the time complexity of the algorithm in Listing 1 by avoiding redundant calculations.

It is easy to see that the most time-consuming steps in this algorithm are the Kronecker product and transitive closure computations. Recall that the matrix \mathcal{M}_2 is always changed in incremental manner i. e. elements (edges) are added to \mathcal{M}_2 (and are never deleted from it) on each iteration of the algorithm in Listing 1. So one does not need to recompute the whole product or transitive closure if an appropriate data structure is maintained.

To deal with the Kronecker product computation, we use the left-distributivity of the Kronecker product. Let \mathcal{A}_2 be a matrix with newly added elements and \mathcal{B}_2 be a matrix with the all previously found elements, such that $\mathcal{M}_2 = \mathcal{A}_2 + \mathcal{B}_2$. Then by the left-distributivity of the Kronecker product we have $\mathcal{M}_1 \otimes \mathcal{M}_2 = \mathcal{M}_1 \otimes (\mathcal{A}_2 + \mathcal{B}_2) = \mathcal{M}_1 \otimes \mathcal{A}_2 + \mathcal{M}_1 \otimes \mathcal{B}_2$. Notice that $\mathcal{M}_1 \otimes \mathcal{B}_2$ is known and is already in the matrix \mathcal{M}_3 and its transitive closure also is already in the matrix C_3 , because it was calculated on the previous iterations, so it is left to update some elements of \mathcal{M}_3 by computing $\mathcal{M}_1 \otimes \mathcal{A}_2$,

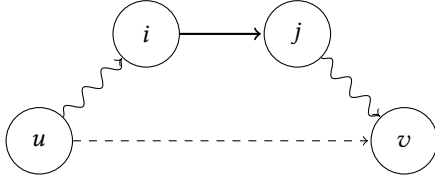


Figure 6: The vertex j become reachable from the vertex u after the addition of edge (i, j) . Then the vertex v is reachable from u after inserting the edge (i, j) if v is reachable from j .

which can be done in $O(|\mathcal{A}_2||M_1|)$ time, where $|\mathcal{A}|$ denotes the number of non-zero elements in a matrix \mathcal{A} .

The fast computation of transitive closure can be obtained by using incremental dynamic transitive closure technique. We use an approach by Ibaraki and Katoh [24] to maintain dynamic transitive closure. The key idea of their algorithm is to recalculate reachability information only for those vertices, which become reachable after insertion of the certain edge (see Figure 6 for details). The algorithm is presented in Listing 3 (we have slightly modified it to efficiently track new elements of the matrix C_3).

Listing 3 The dynamic transitive closure procedure

```

1: function ADD( $C_3, i, j$ )
2:    $n \leftarrow$  Number of rows in  $C_3$ 
3:    $C'_3 \leftarrow$  Empty matrix of size  $n \times n$ 
4:   for  $u \neq 0 \in \text{checkCondition}(C_3, i, j)$  do
5:      $\text{newReachablePairs}(C_3, C'_3, u, j)$ 
6:   return  $C'_3$ 
7: function CHECKCONDITION( $C_3, i, j$ )
8:    $A \leftarrow$  Empty array of size  $n$ 
9:   for  $u \in 0 \dots n \mid u \neq j$  do  $\triangleright 1 \wedge 1 = 0 \wedge 0 = 1 \wedge 0 = 0; 0 \wedge 1 = 1$ 
10:     $A[u] = C_3[u, j] \wedge C_3[u, i]$ 
11:  return  $A$ 
12: function NEWREACHABLEPAIRS( $C_3, C'_3, u, j$ )
13:   $C'_3[u, v] = C_3[u, v] \wedge C_3[j, v] \quad \triangleright 1 \wedge 1 = 0 \wedge 0 = 1 \wedge 0 = 0;$ 
     $0 \wedge 1 = 1$ 

```

Final version of the modified algorithm from Listing 1 is shown in Listing 4.

THEOREM 3.5. *Let $\mathcal{G} = (V, E, L)$ be a graph and $G = \langle \Sigma, N, S, P \rangle$ be a grammar. The algorithm from Listing 4 calculates a result matrices M_2 and C_3 in $O(n^3)$ time where $n = |V|$.*

PROOF. Let $|\mathcal{A}|$ be a number of non-zero elements in a matrix \mathcal{A} . Consider the total time which is needed for computing the Kronecker products. The elements of the matrices $\mathcal{A}_2^{(i)}$ are pairwise distinct on every i -th iteration of the algorithm therefore we have

$$\sum_i T(M_1 \otimes \mathcal{A}_2^{(i)}) = |M_1| \otimes \sum_i |\mathcal{A}_2^{(i)}| = |M_1|O(n^2)$$

Listing 4 Kronecker product based CFPQ using dynamic transitive closure

```

1: function CONTEXTFREEPATHQUERYING( $G, \mathcal{G}$ )
2:    $R \leftarrow$  Recursive automata for  $G$ 
3:    $M_1 \leftarrow$  Adjacency matrix for  $R$ 
4:    $M_2 \leftarrow$  Adjacency matrix for  $\mathcal{G}$ 
5:    $A_2 \leftarrow$  Adjacency matrix for  $\mathcal{G}$ 
6:    $C_3 \leftarrow$  The empty matrix
7:   for  $s \in 0 \dots \text{dim}(M_1) - 1$  do
8:     for  $i \in 0 \dots \text{dim}(M_2) - 1$  do
9:        $M_2[i, i] \leftarrow M_2[i, i] \cup \text{getNonterminals}(R, s, s)$ 
10:  while Matrix  $M_2$  is changing do
11:     $M'_3 \leftarrow M_1 \otimes A_2$ 
12:     $A_2 \leftarrow$  The empty matrix of size  $n \times n$ 
13:    for  $M'_3[i, j] \mid M'_3[i, j] = 1$  do
14:       $C_3[i, j] \leftarrow 1$ 
15:       $C'_3 \leftarrow \bigcup_{(i,j)} \text{add}(C_3, i, j) \triangleright$  Updating the transitive closure
16:       $C_3 \leftarrow C_3 + C'_3$ 
17:     $n \leftarrow \text{dim}(M_3)$ 
18:    for  $(i, j) \mid C'_3[i, j] \neq 0$  do
19:       $s, f \leftarrow \text{getStates}(C'_3, i, j)$ 
20:      if  $\text{getNonterminals}(R, s, f) \neq \emptyset$  then
21:         $x, y \leftarrow \text{getCoordinates}(C'_3, i, j)$ 
22:         $M_2[x, y] \leftarrow M_2[x, y] \cup \text{getNonterminals}(R, s, f)$ 
23:         $A_2[x, y] \leftarrow A_2[x, y] \cup \text{getNonterminals}(R, s, f)$ 
24:  return  $M_2, C_3$ 

```

operations in total.

Now we derive the time complexity of maintaining the dynamic transitive closure. Notice that C_3 has size of $O(n^2)$ so no more than $O(n^2)$ edges will be added during all iterations of the Algorithm. The function *checkCondition* from the Listing 3 takes $O(n)$ time for every inserted edge (i, j) . Thus we have $O(n^2n) = O(n^3)$ operations in total. The function *newReachablePairs* requires $O(n)$ time for a given vertex u . This operation is performed for every pair (j, v) of vertices such that a vertex j became reachable from the vertex u . The vertex j become reachable from the vertex u (and accordingly the value of the matrix cell $C_3[u, j]$ becomes 1 from 0) only once during the entire computation, so the function *newReachablePairs* will be executed at most $O(n^2)$ times for every u and hence $O(n^3)$ times in total for all vertices. Therefore $O(n^3)$ operations are performed to maintain dynamic transitive closure during all iteration of the algorithm from Listing 4.

Notice that the matrix C'_3 contains only new elements, therefore C_3 can be updated directly using only $|C'_3|$ operations and hence $O(n^2)$ operations in total. The same holds for cycle in line 18 of the algorithm from Listing 4, because operations are performed only for non-zero elements of the matrix $|C'_3|$. Finally, we have that the time complexity of the algorithm is $O(n^2) + O(n^3) + O(n^2) + O(n^2) = O(n^3)$. \square

3.1.4 Speeding up by a factor of $\log n$. In this subsection we use the Four Russians' trick to speed up the dynamic transitive closure algorithm from the Listing 3.

THEOREM 3.6. *The computation of transitive closure matrices can be done in $O(n^3/\log n)$ time when n^2 edges are added to the graph.*

PROOF. Consider the function *checkCondition* from the Listing 3. Its operations are equivalent to the element-wise (Hadamard) product of two vectors of size n , where multiplication operation is denoted as \wedge and has the following properties: $1 \wedge 1 = 0 \wedge 0 = 1 \wedge 0 = 0$ and $0 \wedge 1 = 1$. The first vector represents reachability of a given vertex i from other vertices $\{u_1, u_2, \dots, u_n\}$ of the graph and the second vector represents the same for a given vertex j . The function *newReachablePairs* also can be reduced to the computation of the Hadamard product of two vectors of size n for a given u_k . The first vector contains the information whether vertices $\{v_1, v_2, \dots, v_n\}$ of the graph are reachable from a given vertex u_k and the second vector represents the same for a given vertex j . The element-wise product of two vectors can be calculated naively in time $O(n)$ which gives the $O(n^3)$ time for maintaining the transitive closure. Thus, the time complexity of the transitive closure can be reduced by speeding up element-wise product of two vectors of size n .

To achieve this goal, we use the Four Russians' trick. Split each vector into $n/\log n$ parts of size $\log n$. Create a table S such that $S(a, b) = a \wedge b$ where $a, b \in \{0, 1\}^{\log n}$. This takes a time $O(n^2 \log n)$, since there are $2^{\log n} = n$ variants of Boolean vectors of size $\log n$ and hence n^2 pairs of vectors (a, b) in total, and each component takes $O(\log n)$ time. With table S , we can calculate product of two parts of size $\log n$ in constant time. There are $n/\log n$ such parts, so the element-wise product of two vectors of size n can be calculated in time $O(n/\log n)$ with $O(n^2 \log n)$ preprocessing. This gives us a dynamic transitive closure algorithm running in time $O(n^3/\log n)$: both of the functions *checkCondition* and *newReachablePairs* are evaluated no more than $O(n^2)$ times during the whole computation, and each function calculates Hadamard product of two vectors in $O(n/\log n)$ time. \square

Notice that the maintaining of the dynamic transitive closure dominates the cost of the algorithm from Listing 4, therefore we immediately deduce the following.

COROLLARY 3.7. *Let $\mathcal{G} = (V, E, L)$ be a graph and $G = \langle \Sigma, N, S, P \rangle$ be a grammar. The result result matrices \mathcal{M}_2 and C_3 can be calculated in $O(n^3/\log n)$ time.*

Finally, we formulate the theorem which connects the time complexity of CFPQ and time complexity of specific incremental transitive closure of a directed graph.

THEOREM 3.8. *Subcubic incremental transitive closure leads to subcubic CFPQ. Suppose the incremental transitive closure problem where only insertion queries are allowed and the result of each insertion is a set of newly connected pairs. If one can solve this problem in $O(n^{3-\epsilon})$ total time for n^2 insertions, then one can solve CFPQ in $O(n^{3-\epsilon})$, where n is a number of vertices in the graph in both cases.*

3.2 Paths Extraction Algorithm

After index created one can enumerate all paths between specified vertices. Note, that the index stores information about all reachable pairs for all nonterminals. Thus, the most natural way to use this index is to query paths between specified vertices derivable from specified nonterminal.

To do it we provide a function *GETPATHS*(v_s, v_f, N), where v_s is a start vertex of the graph, v_f — the final vertex, and N is a nonterminal. Implementation of this function is presented in Listing 5.

Listing 5 Paths extraction algorithm

```

1:  $C_3 \leftarrow$  result of index creation algorithm: final transitive closure
2:  $\mathcal{M}_1 \leftarrow$  the set of adjacency matrices of the input RSM
3:  $\mathcal{M}_2 \leftarrow$  the set of adjacency matrices of the final graph
4: function GETPATHS( $v_s, v_f, N$ )
5:    $q_N^0 \leftarrow$  Start state of automata for  $N$ 
6:    $F_N \leftarrow$  Final states of automata for  $N$ 
7:    $res \leftarrow \bigcup_{f \in F_N} \text{GETPATHSINNER}((q_N, v_s), (f, v_f))$ 
8:   return  $res$ 
9: function GETSUBPATHS(( $s_i, v_i$ ), ( $s_j, v_j$ ), ( $s_k, v_k$ ))
10:   $l \leftarrow \{(v_i, t, v_k) \mid M_2^t[s_i, s_k] \wedge M_1^t[v_i, v_k]\}$ 
         $\cup \bigcup_{\{N \mid M_2^N[s_i, s_k]\}} \text{GETPATHS}(v_i, v_k, N)$ 
         $\cup \text{GETPATHSINNER}((s_i, v_i), (s_k, v_k))$ 
11:   $r \leftarrow \{(v_k, t, v_j) \mid M_2^t[s_k, s_j] \wedge M_1^t[v_k, v_j]\}$ 
         $\cup \bigcup_{\{N \mid M_2^N[s_k, s_j]\}} \text{GETPATHS}(v_k, v_j, N)$ 
         $\cup \text{GETPATHSINNER}((s_k, v_k), (s_j, v_j))$ 
12:  return  $l \cdot r$ 
13: function GETPATHSINNER(( $s_i, v_i$ ), ( $s_j, v_j$ ))
14:   $parts \leftarrow \{(s_k, v_k) \mid C_3[(s_i, v_i), (s_k, v_k)] = 1 \wedge$ 
         $C_3[(s_k, v_k), (s_j, v_j)] = 1\}$ 
15:  return  $\bigcup_{(s_k, v_k) \in parts} \text{GETSUBPATHS}((s_i, v_i), (s_j, v_j), (s_k, v_k))$ 

```

Paths extraction is implemented as three mutually recursive functions. The entry point is *GETPATHS*(v_s, v_f, N). This function returns a set of paths between v_s and v_f such that the word formed by the path is derivable from nonterminal N .

To compute such paths it is necessary to compute paths from vertices of the form (q_N^s, v_s) to vertices of the form (q_N^f, v_f) in the result of transitive closure, where q_N^s is an initial state of RSM for N and q_N^f is a final state. To do it

GETPATHSINNER($(s_i, v_i), (s_j, v_j)$) is used. This function finds all possible vertices (s_k, v_k) which split path from (s_i, v_i) to (s_j, v_j) into two subpaths. After that, function GETSUBPATHS($(s_i, v_i), (s_j, v_j), (s_k, v_k)$) is used to compute corresponding subpaths. Each part of the path may be a single edge, or path with length more than one. In the second case GETPATHSINNER is used to restore corresponding paths. In the first case, the edge can be labeled by terminal or nonterminal. In the first case corresponding edge should be added to the result. In the second case, GETPATHS should be used to restore paths.

Note, that, first of all, we assume that sets are computed lazily. It is necessary to work correctly in the case of an infinite number of paths. Second, we use a set of path as a result, so we did not check duplicated paths manually.

3.3 An example

In this section we introduce detailed example to demonstrate steps of the proposed algorithms. Our example is based on the classical worst case scenario introduced by Jelle Hellings in [22]. Namely, let we have a graph \mathcal{G} presented in Figure 1 and the RSM R presented in Figure 5.

First step we represent graph as a set of Boolean matrices as presented in Figure 2, and RSM as a set of Boolean matrices as presented in Figure 4. Note, that we should formally add new empty matrix M_2^S to \mathcal{M}_2 , where edges labeled by S will be added in time of the computation.

After the initialization, the algorithm handles ε -case. The input RSM does not have ε -transitions and does not have states that are both start and final, therefore, no edges added at this stage. After that we should iteratively compute \mathcal{M}_2 and C_3 . The loop iteration number of matrices evaluation is provided as the subscript in parentheses.

First iteration. Firstly, we compute Kronecker product of the \mathcal{M}_1 and $\mathcal{M}_{2,(0)}$ matrices and store result in the $\mathcal{M}_{3,(1)}$, and collapse this matrix to the single Boolean matrix $M'_{3,(1)}$. For the sake of simplicity, we provide only $M'_{3,(1)}$, which is evaluated as follows in the equivalent way.

$$M'_{3,(1)} = M_1^a \otimes M_{2,(0)}^a + M_1^b \otimes M_{2,(0)}^b + M_1^S \otimes M_{2,(0)}^S =$$

	(0,0)	(0,1)	(0,2)	(0,3)	(1,0)	(1,1)	(1,2)	(1,3)	(2,0)	(2,1)	(2,2)	(2,3)	(3,0)	(3,1)	(3,2)	(3,3)
(0,0)
(0,1)
(0,2)
(0,3)
(1,0)
(1,1)
(1,2)
(1,3)
(2,0)
(2,1)
(2,2)
(2,3)
(3,0)
(3,1)
(3,2)
(3,3)

As far as the input graph has no edges with label S , therefore, the correspondent block of the Kronecker product will be empty. Then, the transitive closure evaluation result,

stored in the matrix $C_{3,(1)}$, introduces one new path of length 2 (respective cell is filled with a grey colour).

$$C_{3,(1)} = \text{transitiveClosure}(M'_{3,(1)}) =$$

	(0,0)	(0,1)	(0,2)	(0,3)	(1,0)	(1,1)	(1,2)	(1,3)	(2,0)	(2,1)	(2,2)	(2,3)	(3,0)	(3,1)	(3,2)	(3,3)
(0,0)
(0,1)
(0,2)
(0,3)
(1,0)
(1,1)
(1,2)
(1,3)
(2,0)
(2,1)
(2,2)
(2,3)
(3,0)
(3,1)
(3,2)
(3,3)

This path starts in the vertex $(0, 1)$ and finishes in the vertex $(3, 3)$. We can see, that 0 and 3 are a start and a final states of the some component state machine for label S in R respectively. Thus we can conclude that there exists a path between vertices 1 and 3 in the graph, such that respective word is derivable from S in the R execution flow.

As a result, we can add the edge $(1, S, 3)$ to the result graph, what is formally done by the update of the matrix M_2^S .

Second iteration. Modified graph Boolean adjacency matrices contain now edge with label S . Therefore, this label contributes to the non-empty corresponding matrix block in the evaluated matrix $M'_{3,2}$. The transitive closure evaluation introduces three new paths. Since only path between vertices $(0, 0)$ and $(3, 2)$ connects start and final states if the automata, the edge $(0, S, 2)$ is added to the result graph.

$$M'_{3,(2)} = M_1^a \otimes M_{2,(2)}^a + M_1^b \otimes M_{2,(2)}^b + M_1^S \otimes M_{2,(2)}^S =$$

	(0,0)	(0,1)	(0,2)	(0,3)	(1,0)	(1,1)	(1,2)	(1,3)	(2,0)	(2,1)	(2,2)	(2,3)	(3,0)	(3,1)	(3,2)	(3,3)
(0,0)
(0,1)
(0,2)
(0,3)
(1,0)
(1,1)
(1,2)
(1,3)
(2,0)
(2,1)
(2,2)
(2,3)
(3,0)
(3,1)
(3,2)
(3,3)

$$C_{3,(2)} = \text{transitiveClosure}(M'_{3,(2)}) =$$

	(0,0)	(0,1)	(0,2)	(0,3)	(1,0)	(1,1)	(1,2)	(1,3)	(2,0)	(2,1)	(2,2)	(2,3)	(3,0)	(3,1)	(3,2)	(3,3)
(0,0)
(0,1)
(0,2)
(0,3)
(1,0)
(1,1)
(1,2)
(1,3)
(2,0)
(2,1)
(2,2)
(2,3)
(3,0)
(3,1)
(3,2)
(3,3)

The result transitive closure matrix $C_{3,(6)}$ of the remaining iterations evaluated as follows. The result graph is presented in figure 7.

first. It is possible, for example one can use existing proposal⁵ to extend Cypher language, but it requires a lot of technical effort, so it is an interesting challenge for future research to provide full-stack support for CFPQ.

Paths extraction also is implemented in Python by using PyGraphBLAS. For evaluation we implement a version which has an additional parameter: a maximal number of paths to extract. This modification allows as to avoid lazy evaluation which is not natural for Python. Note that one can provide other modifications of paths extraction algorithm based on the proposed idea.

5 EVALUATION

We evaluate the implemented algorithm on both regular and context-free path queries in order to demonstrate applicability of the proposed solution. Namely, goals of the evaluation are following.

- (1) Investigate practical applicability of RPQ evaluation by the proposed algorithm.
- (2) Compare Azimov's algorithm for reachability CFPQ and the proposed algorithm.
- (3) Investigate practical applicability of paths extraction algorithm for both regular and context-free queries.

For evaluation, we use a PC with Ubuntu 18.04 installed. It has Intel core i7-6700 CPU, 3.4GHz, and DDR4 64Gb RAM. As far as we evaluate only algorithm execution time, we store each graph fully in RAM as its adjacency matrix in sparse format. Note, that graph loading time is not included in the result time of evaluation.

5.1 RPQ Evaluation

In order to investigate applicability of the proposed algorithm for RPQ over real-world graphs we collect a set of real-world and synthetic graphs and evaluate queries generated by using the most popular templates for RPQs.

5.1.1 Dataset. Brief description of collected graphs are presented in table 1. Namely, the dataset consists of several parts. The first one is a set of LUBM graphs⁶ [19] with different number of vertices. The second one is a graphs from Uniprot database⁷: *proteomes*, *taxonomy* and *uniprotkb*. The last part is a RDF files *mappingbased_properties* from DBpedia⁸ and

⁵Cypher language extension proposal which introduces a syntax to express context-free queries: <https://github.com/thobe/openCypher/blob/rpq/cip/1.accepted/CIP2017-02-06-Path-Patterns.adoc>. Access date: 07.07.2020.

⁶Lehigh University Benchmark (LUBM) web page: <http://swat.cse.lehigh.edu/projects/lubm/>. Access date: 07.07.2020.

⁷Universal Protein Resource (UniProt) web page: <https://www.uniprot.org/>. All files used for evaluation can be downloaded here: ftp://ftp.uniprot.org/pub/databases/uniprot/current_release/rdf/. Access date: 07.07.2020.

⁸DBpedia project web site: <https://wiki.dbpedia.org/>. Access date: 07.07.2020.

Graph	#V	#E
LUBM100	300000	4000000
LUBM300	3	4
LUBM500	3	4
LUBM1M	3	4
LUBM1.5M	3	4
LUBM1.9M	3	4
Uniprotkb	3	4
Proteomes	3	4
Taxonomy	3	4
Geospecies	3	4
Mappingbased_properties	3	4

Table 1: Graphs for RPQ evaluation

Name	Query	Name	Query
q_1	a^*	q_9_5	$(a b c d e)^+$
q_2	$a \cdot b^*$	q_10_2	$(a b) \cdot c^*$
q_3	$a \cdot b^* \cdot c^*$	q_10_3	$(a b c) \cdot d^*$
q_4_2	$(a b)^*$	q_10_4	$(a b c d) \cdot e^*$
q_4_3	$(a b c)^*$	q_10_5	$(a b c d e) \cdot f^*$
q_4_4	$(a b c d)^*$	q_10_2	$a \cdot b$
q_4_5	$(a b c d e)^*$	q_11_3	$a \cdot b \cdot c$
q_5	$a \cdot b^* \cdot c$	q_11_4	$a \cdot b \cdot c \cdot d$
q_6	$a^* \cdot b^*$	q_11_5	$a \cdot b \cdot c \cdot d \cdot f$
q_7	$a \cdot b \cdot c^*$	q_12	$(a \cdot b)^+ (c \cdot d)^+$
q_8	$a? \cdot b^*$	q_13	$(a \cdot (b \cdot c)^*)^+ (d \cdot f)^+$
q_9_2	$(a b)^+$	q_14	$(a \cdot b \cdot (c \cdot d)^*)^+ \cdot (e f)^*$
q_9_3	$(a b c)^+$	q_15	$(a b)^+ \cdot (c d)^+$
q_9_4	$(a b c d)^+$	q_16	$a \cdot b \cdot (c d e)$

Table 2: Queries' templates for RPQ evaluation

*geospecies*⁹. These graphs represents data from different areas and they are frequently used for graph querying algorithms evaluation.

Queries for evaluation was generated by using templates of the most popular RPQs which are collected from [36] (Table 2) and [46] (some of complex queries from Table 5), and are presented in table 2. We generate 10 queries for each template and each graph using the most frequent relations from the given graph randomly¹⁰. For all LUBM graphs common set of queries was generated in order to investigate scalability of the proposed algorithm.

5.1.2 Results. Results of evaluation

⁹The Geospecies RDF: <https://old.datahub.io/dataset/geospecies>. Access date: 07.07.2020.

¹⁰Used generator is available as part of CFPQ_data project: https://github.com/JetBrains-Research/CFPQ_Data/blob/master/tools/gen_RPQ/gen.py. Access data: 07.07.2020.

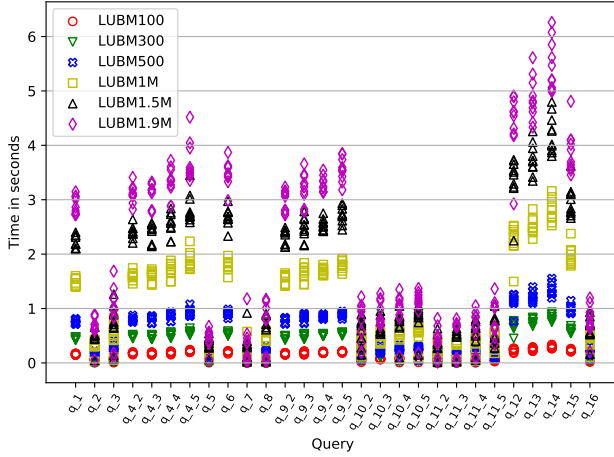


Figure 9: Reachability index creation time for LUBM series

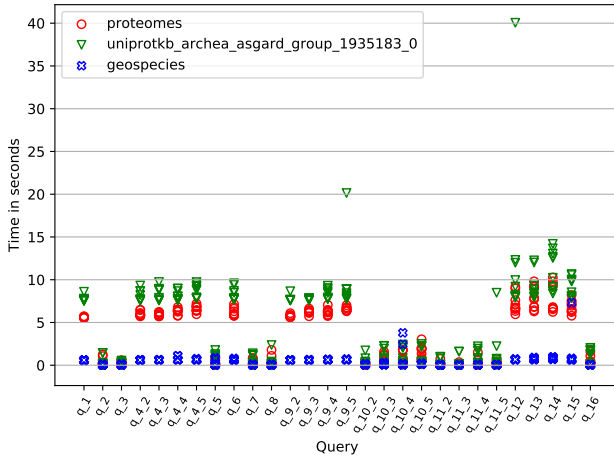


Figure 10: Reachability index creation time for real-world RDFs

Reachability index creation time for each query for LUBM graphs set is presented in figure 9. We can observe linear dependency of evaluation time on graph size. Also we can see, that query evaluation time depends on query: there are queries which evaluate less then 1 second even for biggest graph (q_2, q_5, q_11_2, q_11_3), while worst time is 6.26 seconds (q_14). Anyway, we can argue that in this case our algorithm demonstrates reasonable time to be applied for real-world data analysis, because !!!!

Reachability index creation time for each query for for real-world graphs is presented in figure 10.

Paths extraction was evaluated on cases with possible long paths. These cases were selected during reachability index

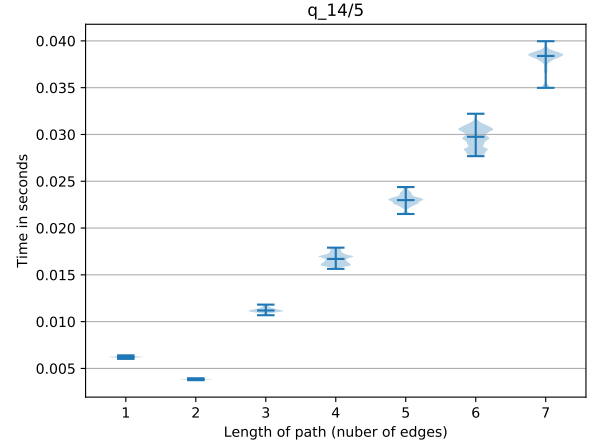


Figure 11: Single path extraction

creation by using number of iterations in transitive closure evaluation. For each selected graph and query we measure paths extraction time for each reachable pair.

We evaluate two scenarios. The first one is a single path extraction. In this case results are represented as a dependency of extraction time on extracted path length. We can see linear !!!!

The second scenario is many paths extraction. Here we limit a number of path to extract by !!! In this case results are represented as a dependency of extraction time on number of extracted paths.

5.1.3 Conclusion.

5.2 CFPQ Evaluation

Comparison with matrix-based algorithm.

5.2.1 Dataset. Dataset for evaluation. It should be CFPQ_Data¹¹ Same-generation queries, memory aliases.

5.2.2 Results. Results of evaluation.

Index creation.

Paths extraction.

5.2.3 Conclusion.

6 RELATED WORK

Language constrained path querying widely used in graph databases, static code analysis and other areas. Both, RPQ and CFPQ (known as CFL reachability problem in static code analysis) actively studied last years.

¹¹CFPQ_Data is a dataset for CFPQ evaluation which contains both synthetic and real-world data and queries https://github.com/JetBrains-Research/CFPQ_Data. Access date: 07.07.2020.

There is a huge number of theoretical research on RPQ and its specific cases. RPQ with single-path semantics was investigated from theoretical point of view by Barrett et al. in [5]. In order to research practical limits and restrictions of RPQ, a number of high-performance RPQ algorithms were provided. For example, derivative-based solution provided by Maurizio Nol  and Carlo Sartiani which is implemented on the top of Pregel-based system [35], or solution of Andr  Koschmieder et al. [27]. But only limited number of practical solutions provide ability to restore paths of interest. One of the recent work is a research of Xin Wang et al. [46] in which Pregel-based provenance-aware RPQ algorithm, which utilizes a Glushkov's construction [17], is provided. Applicability of linear algebra based RPQ algorithms with paths-providing semantics is not investigated.

On the other hand, a bunch of CFPQ algorithms based on different ideas and with different properties was proposed in recent years. All of them have not better than cubic time complexity in terms of input graph size, and exploit ideas of different parsing algorithms, such as CYK in works of Jelle Hellings [21] and Phillip Bradford [7], (G)LR and (G)LL in works of Ekaterina Verbitskaia et al. [45], Semyon Grigorev et al. [18], Fred Santos et al. [38], Ciro Medeiros et al. [32]. Worth mentioning separately Azimov's algorithm [3], which is first, in our knowledge, linear-algebra based algorithm for CFPQ. It was shown by Arseniy Terekhov et al. [42] that this algorithm can be applied for real-world graph analysis problems, while Jochem Kuijpers et al. shows in [29] that other state-of-the-art CFPQ algorithms are not performant enough to handle real-world graphs.

One of the important properties of both RPQ and CFPQ algorithms is an ability to restore paths of interest. Some of mentioned algorithms can solve only reachability problem, while in some cases it is important to provide at least one path satisfies query. While Arseniy Terekhov et al. [42] provide first linear algebra based CFPQ algorithm with single path semantics, Jelle Hellings in [?] provides first theoretical investigation of this problem. Also he provide overview of related researches and shows that the problem is related to strings generation problem and respective results from formal language theory. Also he conclude that both theoretical and empirical investigation of CFPQ with single-path and all-path semantics are in early stage, and we agree with this point of view, because we only demonstrates applicability of our solution on paths extraction, without detailed investigation of its properties.

Subcubic CFPQ is a long-standing problem which is actively studied in both graph database and static code analysis communities. The question on existence of subcubic CFPQ algorithm was asked by Mihalis Yannakakis in 1990 in [47]. He notes that Valiant's algorithm [43], the first known truly

subcubic algorithm for context-free parsing, can be generalized to direct acyclic graph querying, but it unlikely can be applied for general CFPQ. A bit later Thomas Reps propose a CFL reachability as a framework for interprocedural static code analysis formulate a problem of subcubic bottleneck of context-free language reachability [?]. Since these problems were formulated,!!!! The most general result is a slightly subcubic algorithm inspired by recursive state machine reachability, which was provided by Swarat Chaudhuri in [13]. This algorithm achieve logarithmic speedup and thus $O(n^3/\log n)$ time complexity. The first truly subcubic algorithm with $\tilde{O}(n^\omega)$ time complexity (ω is the best exponent for matrix multiplication, \tilde{O} is the asymptotic upper-bound mod polylog factors) for general graph and 1-Dyck language was provided by Phillip Bradford in [8]. Unfortunately, this result cannot be generalized to general context-free queries. The similar result was provided by Andreas Pavlogiannis and Anders Alnor Mathiasen in [37]. Another partial case was investigated by Krishnendu Chatterjee et al. in [11]. The $O(m + n \cdot \alpha(n))$ algorithm for an arbitrary Dyck querying of bidirected graph was described. Here m is a number of edges, n is a number of vertices in the input graph, and $\alpha(x)$ is an inverse Ackermann function. Specific types of static code analysis related to CFL-r, especially Andersen's Pointer Analysis also actively studying. For example, recently BMM-hardness of 1-Dyck reachability was proven by Qirun Zhang in [48]. Other partial cases such as tree querying also were studied.

Utilization of linear algebra is a promising way to high-performance graph analysis. There is a big number of works on specific graph algorithm formulation in terms of linear algebra, for example classical algorithms for transitive closure and all pairs shortest paths. Recently this direction was summarized in GrpahBLAS API [26] which provide building blocks to develop graph analysis algorithm in terms of linear algebra. There is a number of implementation of this API, such as SuiteSparse:GraphBLAS [15] or CombBLAS [9]. Also, linear algebra based approaches to evaluate different classes of queries in different systems actively studying. This approach demonstrates significant performance improvement when applied for SPARQL queries evaluation [25, 33] and for Datalog queries evaluation [39]. Finally, RedisGraph [10], a linear-algebra powered graph database, was created, and it was shown that it outperforms many other graph databases in some scenarios.

7 CONCLUSION AND FUTURE WORK

In this work we present an improved version of the tensor-based algorithm for CFPQ: we reduce the algorithm to operations over Boolean matrices, and we provide ability to extract all paths which satisfy the query. Moreover, the provided

algorithm can handle grammars in EBNF, thus it does not require grammar to be in CNF transformation and avoids grammar explosion. As a result, the algorithm demonstrates practical performance not only on CFPQ queries, but also on RPQ ones, which shown by our evaluation. Thus, we provide universal linear algebra based algorithm for RPQ and CFPQ evaluation with all-paths semantics.

The first important task for the future research is an detailed investigation of paths extraction algorithm. Jelle Hellings in [?] provides theoretical investigation of single path extraction, and shows that the problem is related to formal language theory. All paths extraction is more complicated and should be investigated carefully in order to provide optimal algorithm.

Also the algorithm open a way to attack long-standing problem on subcubic CFPQ by reducing it to incremental transitive closure: *incremental transitive closure with $O(n^{3-\epsilon})$ total update time for n^2 updates, such that each update returns all new reachable pairs, implies $O(n^{3-\epsilon})$ CFPQ algorithm.* In this work we prove $O(n^3/\log n)$ time complexity by providing $O(n/\log n)$ transitive closure algorithm.

Thus, the first task for the future is to find truly sublinear algorithm for incremental transitive closure or, as a first step, to improve logarithmic factor. Also, it is interesting to get improved bounds in partial cases. For example, fully dynamic transitive closure for planar graphs can be supported in $O(n^{2/3} \log n)$ time per update [41], and for undirected graph one can use *disjoint sets* which provide operations with time complexity bounded by inverse Ackermann function. Can we use these facts to provide better CFPQ algorithm for respective partial cases? In the case of planarity it is interesting to investigate properties of the input graph and grammar which allow to preserve planarity during query evaluation.

On the other hand, provided reduction open a way to investigate streaming graph querying. This way we can formulate the following questions.

- (1) Can we provide more detailed analysis of dynamic CFPQ queries, than provided in [6]?
- (2) Can we provide practical solution for CFPQ querying of streaming graphs?
- (3) Can we improve existing solutions for RPQ of streaming graphs?

From a practical perspective, it is necessary to analyze the usability of advanced algorithms for dynamic transitive closure. In the current work we evaluate naïve implementation in which transitive closure recalculated on each iteration from scratch. In [20] it is shown that some of advanced algorithms for dynamic transitive closure can be efficiently implemented. Can one of these algorithms be efficiently parallelized and utilized in the proposed algorithm?

Also, it is necessary to evaluate GPGPU-based implementation. Experience in Azimov's algorithm shows that the utilization of GPGPUs allows one to improve performance because operations of linear algebra can be efficiently implemented on GPGPU [34, 42]. Moreover, for practical reason, it is interesting to provide a multi-GPU version of the algorithm and to utilize unified memory, which is suitable for linear algebra based processing of out-of-GPGPU-memory data and traversing on large graphs [14, 16].

In order to simplify the distributed processing of huge graphs, it may be necessary to investigate different formats for sparse matrices, such as HiCOO format [30]. Another interesting question in this direction is about utilization of virtualization techniques: should we implement distributed version of algorithm manually or it can be better to use CPU and RAM virtualization to get a virtual machine with huge amount of RAM and big number of computational cores. The experience of the Trinity project team shows that it can make sense [40].

Finally, it is necessary to provide a multiple-source version of the algorithm and integrate it with a graph database. RedisGraph¹² [10] is a suitable candidate for this purpose. This database uses SuiteSparse—an implementation of Graph-BLAS standard—as a base for graph processing. This fact allowed to Arseny Terkhov et.al. to integrate Azimov's algorithm to RedisGraph with minimal effort [42].

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¹²RedisGraph is a graph database that is based on the Property Graph Model. Project web page: <https://oss.redislabs.com/redisgraph/>. Access date: 07.07.2020.

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