Context-Free Path Querying by Kronecker Product*

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Abstract. Context-free path queries (CFPQ) extend regular path queries (RPQ) by allowing context-free grammars to be used as constraints for paths. Algorithms for CFPQ are actively developed, but J. Kuijpers et al. have recently concluded, that existing algorithms are not performant enough to be used in real-world applications. Thus the development of new algorithms for CFPQ is justified. In this paper, we provide a new CFPQ algorithm which is based on such linear algebra operations as Kronecker product and transitive closure and handles grammars presented as recursive state machines. Thus, the proposed algorithm can be implemented by using high-performance libraries and modern parallel hardware. Moreover it avoids grammar growth which provides the possibility for queries optimization.

Keywords: Context-free path querying · Graph database · Context-free grammars · CFPQ · Kronecker product · Recursive state machines.

1 Introduction

Language-constrained path querying [3], and particularly context-free path querying (CFPQ) [13], allows one to express constraints for paths in a graph in terms of context-free grammars. A path in a graph is included into a query result only if the labels along this path form a word which belongs to the language, generated by the query grammar. CFPQ is widely used in bioinformatics [12], graph databases querying [5, 10, 9], and RDF analysis [14].

CFPQ algorithms are actively developed, but still suffer from poor performance [9]. The algorithm proposed by Rustam Azimov [2] is one of the most promising. This algorithm makes it possible to offload computational intensive computations to high-performance libraries for linear algebra, this way one can utilize modern parallel hardware for CFPQ. One disadvantage of this algorithm

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is that a query grammar should be converted to a Chomsky Normal Form (CNF) which significantly increases its size. Performance of the algorithm depends on the grammar size, thus it is desirable to create the algorithm which does not modify the query grammar.

In this work, we propose a new algorithm for CFPQ which can be expressed in terms of matrix operations and does not require grammar transformation. This algorithm can be efficiently implemented on modern parallel hardware and it provides ways to optimize queries. The main contribution of this paper could be summarized as follows.

1. We introduce a new algorithm for CFPQ, which is based on the intersection of recursive state machines and can be expressed in terms of Kronecker product and transitive closure.
2. We provide a step-by-step example of the algorithm.
3. We provide an evaluation of the presented algorithm and its comparison with the matrix-based algorithm. The presented algorithm outperformes the previous matrix-based algorithm in the worst-case scenario, but further optimizations are required to make it applicable for real-world cases.

2 Recursive State Machines

In this section, we introduce the recursive state machine (RSM). This kind of computational machine extends the definition of finite state machines and increases the computational capabilities of this formalism.

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

- M is a finite set of boxes' labels
- 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 set of symbols, $\Sigma \cap M = \emptyset$
  - Q_i is finite set of states, where $Q_i \cap Q_j = \emptyset, \forall i \neq j$
  - q_i^0 is an initial state for component state machine C_i
  - F_i is set of final states for C_i, where $F_i \subseteq Q_i$
  - δ_i is transition function for C_i, where $\delta_i : Q_i \times (\Sigma \cup M) \to Q_i$

RSM behaves as set of finite state machines (or FSM), so called *boxes* or *component state machines* [1], which are executed in classical definition of FSM with additional *recursive calls* and implicit *call stack*, what allows to *call* one component from another, and then return execution flow back.

Accordingly to [1], recursive state machines are equivalent to pushdown systems. Since pushdown systems are capable of accepting context-free languages [7], it is clear that RSMs are equals to context-free languages. Thus we can use an RSMs to encode query grammar. Any CFG can be easily converted to the corresponding RSM with one box per nonterminal. The box corresponding to the nonterminal A constructed using all right hand sides of the rules with

A as left hand side. An example of such RSM R for the grammar G with rule $S \to aSb \mid ab$ is provided in figure 1.

Since R is a set of FSMs, it is useful for computational tasks to represent R as a adjacency matrix, 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 our machine R is be provided in section 3.1.

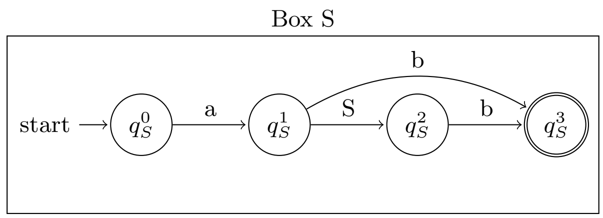


Fig. 1: The recursive state machine R for grammar G

3 Kronecker Product Based CFPQ Algorithm

In this section, we introduce an algorithm for the computation of context-free reachability in a graph $\mathcal{G}$ and an RSM R. The algorithm is based on the generalization of the FSM intersection for an RSM, created from an input grammar, and an input graph. Since a graph can be interpreted as FSM, where edges with labels represent transitions between vertices of the graph, and an RSM is composed of a set of FSMs, it is clear to evaluate the intersection of such machines using the classical algorithm for FSM, represented in [7].

The result of the intersection could be evaluated as a Kronecker product of the corresponding adjacency matrices for RSM and graph. To solve the reachability problem it is enough to represent intersection result as a Boolean matrix because we are interested only in the reachability of vertices. It simplifies algorithm implementation and allows to express it in terms of basic matrix operations.

Listing 1 shows main steps of the solution. As an input algorithm accepts context-free grammar $G = (\Sigma, N, P)$ and graph $\mathcal{G} = (V, E, L)$. RSM R is created from G. Note, that R must have no ε-transitions. M_1 and M_2 are the adjacency matrices for machine R and graph $\mathcal{G}$ correspondingly.

Then for each vertex i of the graph $\mathcal{G}$, the algorithm adds loops with nonterminals, which allows deriving ε-word. Here the rule is implied: each vertex of the graph is reachable by itself through ε-transition. Since the machine R does not have ε-transitions, the ε-word could be derived only if a state s in the box B of the R is initial and final at the same time. This info is queried by $getNonterminals()$ function for each state s.

The algorithm is executed while matrix M_2 is changing. For each iteration Kronecker product of matrices M_1 and M_2 is evaluated. The result is saved in M_3

as a Boolean matrix. For given M_3 evaluated C_3 matrix via $transitiveClosure()$ function call. The M_3 could be interpreted as an adjacency matrix for an oriented graph without labels, used to evaluate transitive closure in terms of classical graph definition of this operation. Then the algorithm iterates over cells of the C_3. For pair of indices (i, j) computes s and f — initial and final states in recursive automata R which relate to the concrete $C_3[i, j]$ of the closure matrix. If given s and f belongs to a same box B of R and $s = q_B^0$ and $f \in F_B$, then $getNonterminals()$ returns the respective non-terminal. If the conditional statement is $true$ then algorithm adds computed non-terminals to the respective cell of the adjacency matrix M_2 of the graph.

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

The algorithm returns updated matrix M_2 which contains initial graph $\mathcal{G}$ data and non-terminals from N. If a cell $M_2[i, j]$ for any valid indices i and j contains symbol $S \in N$, therefore, vertex j is reachable from vertex i in grammar G for non-terminal S.

Listing 1 Kronecker product based CFPQ

```
function CONTEXTFREEPATHQUERYING(G, 𝒢)
    R ← Recursive automata for G
    M1 ← Adjacency matrix for R
    M2 ← Adjacency matrix for 𝒢
    for s ∈ 0..dim(M1) − 1 do
        for i ∈ 0..dim(M2) − 1 do
            M2[i, i] ← M[i, i]2 ∪ getNonterminals(R, s, s)
    while Matrix M2 is changing do
        M3 ← M1 ⊗ M2                                  ▷ Evaluate Kroncker product
        C3 ← transitiveClosure(M3)
        n ← dim(M3)                                   ▷ Matrix M3 size = n × n
        for i ∈ 0..n − 1 do
            for j ∈ 0..n − 1 do
                if C3[i, j] then
                    s, f ← getStates(C3, i, j)
                    if getNonterminals(R, s, f) ≠ ∅ then
                        x, y ← getCoordinates(C3, i, j)
                        M2[x, y] ← M2[x, y] ∪ getNonterminals(R, s, f)
    return M2
```

3.1 Example

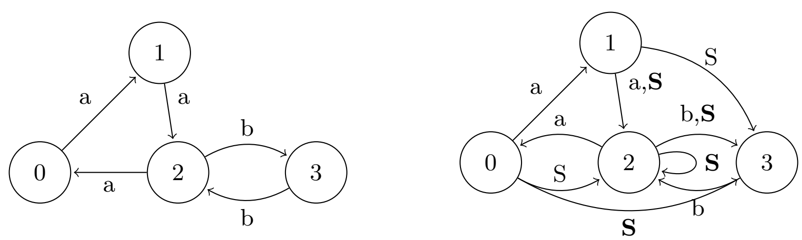
This section is intended to provide a step-by-step demonstration of the proposed algorithm. As an example consider the theoretical worst case for CFPQ

Listing 2 Help functions for Kronecker product based CFPQ

```
1: function getStates(C, i, j)
2:     r ← dim(M_1)                     ▷ M_1 is adjacency matrix for automata R
3:     return ⌊i/r⌋, ⌊j/r⌋
4: function getCoordinates(C, i, j)
5:     n ← dim(M_2)                     ▷ M_2 is adjacency matrix for graph 𝒢
6:     return i mod n, j mod n
```

time complexity, proposed by J.Hellings [5]: graph $\mathcal{G}$ presented in Figure 2a and context-free grammar G for a language $\{a^n b^n \mid n \geq 1\}$: $S \to aSb \mid ab$.

Since the proposed algorithm processes grammar in form of recursive machine, we first provide RSM R in Figure 1. The initial box of the R is S, the initial state q_S^0 is (0), the set of final states $F_S = \{(3)\}$.



(a) The input graph $\mathcal{G}$

(b) The result graph $\mathcal{G}$

Fig. 2: The input and result graphs for example

Adjacency matrices M_1 and M_2 for automata R and graph $\mathcal{G}$ respectively are initialised as follows:

$$M_1 = \begin{pmatrix} . & . & \{a\} & . \\ . & . & \{S\} & \{b\} \\ . & . & . & \{b\} \\ . & . & . & . \end{pmatrix}, \qquad M_2^0 = \begin{pmatrix} . & \{a\} & . & . \\ . & . & \{a\} & . \\ \{a\} & . & . & \{b\} \\ . & . & \{b\} & . \end{pmatrix}.$$

After all the data is initialized in lines **2–4**, the algorithm handles ε-case. Because machine R does not have ε-transitions and ε-word is not included in grammar G language lines **5–7** of the algorithm do not affect the input data.

Then the algorithm enters while loop and iterates as long as matrix M_2 is changing. We provide step-by-step evaluation of matrices M_3, C_3 and updating of matrix M_2. All the matrices are denoted with an upper index of the current loop iteration. The first loop iteration is indexed as 1.

For the first while loop iteration the Kronecker product $M_3^1 = M_1 \otimes M_2^0$ and transitive closure C_3^1 are evaluated as follows:

$$M_3^1 = \left(\begin{array}{cccc|cccc|cccc|cccc}
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\end{array}\right), \quad
C_3^1 = \left(\begin{array}{cccc|cccc|cccc|cccc}
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\end{array}\right).$$

After the transitive closure evaluation $C_3^1[1, 15]$ contains non-zero value. It means that vertex with index 15 is accessible from vertex with index 1 in a graph, represented by adjacency matrix M_3^1.

Then the lines **14–18** are executed. In that section, the algorithm adds non-terminals to the graph matrix M_2^1. Because this step is additive we are only interested in newly appeared values in matrix C_3^1 such as value $C_3^1[1, 15]$ for which we get the following:

- Indices of the automata vertices $s = 0$ and $f = 3$, because value $C_3^1[1, 15]$ located in upper right matrix block $(0, 3)$.
- Indices of the graph vertices $x = 1$ and $y = 3$ are evaluated as value $C_3^1[1, 15]$ indices relatively to its block $(0, 3)$.
- Function $getNonterminals()$ returns $\{S\}$ since this is the only non-terminal which could be derived in path from vertex 0 to 3 in the box S.

Thus we can conclude that the vertex with $id = 3$ is rachable from the vertex with $id = 1$ by path derivable from S. As a result, S is added to the $M_2^1[1, 3]$. The updated matrix and graph after first loop iteration are presented in figure 3.

$$M_2^1 = \begin{pmatrix} . & \{a\} & . & . \\ . & . & \{a\} & \{\mathbf{S}\} \\ \{a\} & . & . & \{b\} \\ . & . & \{b\} & . \end{pmatrix}$$

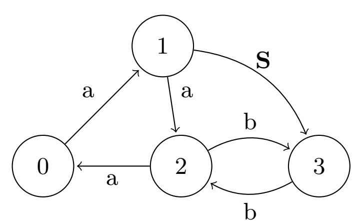

Fig. 3: The updated matrix M_2^1 and graph $\mathcal{G}$ after first loop iteration for example query

For the second loop iteration matrices M_3^2 and C_3^2 are evaluated as follows:

$$M_3^2 = \left(\begin{array}{cccc|cccc|cccc|cccc}
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\end{array}\right), C_3^2 = \left(\begin{array}{cccc|cccc|cccc|cccc}
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\end{array}\right).$$

For this iteration in the matrix C_3^2 appeared new non-zero values in cells with indices $[0,11]$, $[0,14]$ and $[5,14]$. Because only the cell value with index $[0,14]$ corresponds to the automata path with not empty non-terminal set $\{S\}$ its data affects adjacency matrix M_2. The updated matrix and graph $\mathcal{G}$ are depicted in Figure 4.

$$M_2^2 = \begin{pmatrix} . & \{a\} & \{\mathbf{S}\} & . \\ . & . & \{a\} & \{S\} \\ \{a\} & . & . & \{b\} \\ . & . & \{b\} & . \end{pmatrix}$$

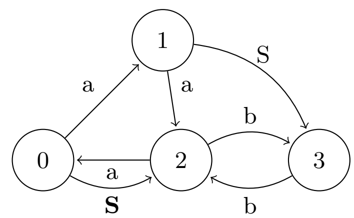

Fig. 4: The updated matrix M_2^2 and graph $\mathcal{G}$ after second loop iteration for example query

The remaining matrices C_3 and M_2 for the algorithm's main loop execution are listed in the Figure 5 and Figure 6 correspondingly. Evaluated matrices M_3 are not included because its computation is a straightforward process. The last loop iteration is 7. Although the matrix M_2^6 is updated with new non-terminal S for the cell $[2,2]$ after transitive closure evaluation the new values to the matrix M_2 are not added. Therefore matrix M_2 has stopped changing and the algorithm is successfully finished. The graph $\mathcal{G}$ with new edges is presented in the Figure 2b.

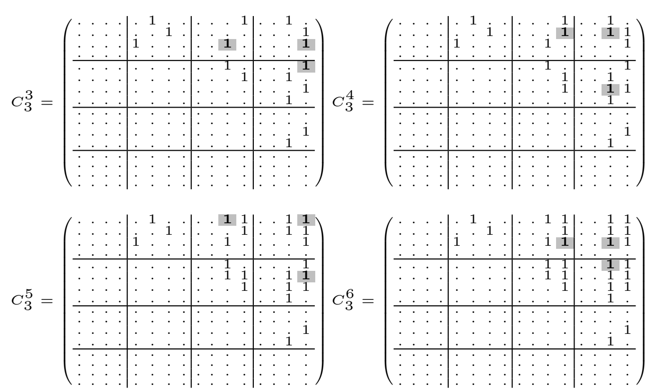

Fig. 5: Transitive closure for $3-6$ loop iterations for example query

$$M_2^3 = \begin{pmatrix} . & \{a\} & \{S\} & . \\ . & . & \{a\} & \{S\} \\ \{a\} & . & . & \{b, \mathbf{S}\} \\ . & . & \{b\} & . \end{pmatrix} M_2^4 = \begin{pmatrix} . & \{a\} & \{S\} & . \\ . & . & \{a, \mathbf{S}\} & \{S\} \\ \{a\} & . & . & \{b, S\} \\ . & . & \{b\} & . \end{pmatrix}$$

$$M_2^5 = \begin{pmatrix} . & \{a\} & \{S\} & \{\mathbf{S}\} \\ . & . & \{a, S\} & \{S\} \\ \{a\} & . & . & \{b, S\} \\ . & . & \{b\} & . \end{pmatrix} M_2^6 = \begin{pmatrix} . & \{a\} & \{S\} & \{S\} \\ . & . & \{a, S\} & \{S\} \\ \{a\} & . & \{\mathbf{S}\} & \{b, S\} \\ . & . & \{b\} & . \end{pmatrix}$$

Fig. 6: The updated matrix M_2 for $3-6$ loop iterations for example query

4 Evaluation

We implement the proposed algorithm by using SuiteSparse[3] [4]: the implementation of GraphBlas API [8]. GraphBlas API specifies a set of linear algebra primitives and operation which allows one to formulate graph algorithms using linear algebra over custom semirings.

We compare our implementation with results provided in [11], accordingly we use dataset described in this article which consists of **RDF**, **Worst case**, and **Full** subsets. For RDF querying we use same-generatoin query G_4 from [11].

For evaluation, we use a PC with Ubuntu 18.04 installed. It has Intel(R) Core(TM) i7-4790 CPU @ 3.60GHz CPU, DDR4 32 Gb RAM.

The results of the evaluation are summarized in the table 1. Time is measured in seconds, t_1 is an execution time for the proposed algorithm, and t_2 is a time for M4RI-based implementation — the best CPU version form [11]. The result for the algorithm is averaged over 10 runs. We exclude the time required to load data from a file. The time required for data transfer and its conversion is included.

Table 1: Evaluation results

	Graph	#V	#E	t_1	t_2		Graph	#V	#E	t_1	t_2
RDF	atm-prim	291	685	0.24	0.02	RDF	core	1323	8684	0.28	0.12
	biomed	341	711	0.24	0.05		wine	733	2450	1.71	0.06
	foaf	256	815	0.07	0.02	Worst case	WC_1	64	65	0.03	0.04
	funding	778	1480	0.43	0.07		WC_2	128	129	0.16	0.23
	generations	129	351	0.04	0.03		WC_3	256	257	0.96	1.99
	people_pets	337	834	0.18	0.03		WC_4	512	513	7.14	23.21
	pizza	671	2604	1.14	0.08		WC_5	1024	1025	121.99	528.52
	skos	144	323	0.02	0.04	Full	F_1	100	100	0.17	0.02
	travel	131	397	0.05	0.05		F_2	200	200	1.04	0.03
	unv-bnch	179	413	0.05	0.04		F_3	500	500	18.86	0.03
	pathways	6238	37196	4.88	0.18		F_4	1000	1000	554.22	0.07

[3] SuteSparse is a sparse matrix software which incudes GraphBLAS API implementation. Project web page: http://faculty.cse.tamu.edu/davis/suitesparse.html. Access date: 12.03.2020

We can see, that while RDF querying time is better for M4RI in general, in some cases execution times are comparable. For example, for graphs *generations*, *travel*, *unv-bnch*, *skos*. For **Full** data set performance of our algorithm is bad because SuiteSparse is based on sparse matrix representation, and in this case matrices density changes aggressively from very sparse to full. At the same time, we can see, that in **Worst case** our algorithms up to 4 times faster than M4RI (graph WC_5).

To sum up, our prototype implementation of the described algorithm is not performant enough to be used for real-world applications but it outperforms a matrix-based algorithm on **Worst case** dataset and comparable with it on some graphs from the **RDF** dataset. Thus we can conclude that we should improve our implementation to achieve better performance.

5 Conclusion

We presented a new algorithm for CFPQ which is based on Kronecker product and transitive closure. Thus it can be implemented by using high-performance libraries for linear algebra. Also, our algorithm handles queries represented as recursive state machines, thus it avoids grammar growth.

We implement the proposed algorithm by using SuiteSparse and evaluate it on several graphs and queries. We show that in some cases our algorithm outperforms the matrix-based algorithm, but in the future, we should improve our implementation to be applicable for real-world graphs analysis.

Also in the future, we should investigate such formal properties of the proposed algorithm as time and space complexity. Moreover, we should analyze behavior dependency on query type and its form. Namely, we should analyze regular path queries evaluation and context-free path queries in the form of extended context-free grammars (ECFG) [6]. Utilization of ECFGs may provide a way to optimize queries by minimization of both the right parts of productions and whole result RSM.

Finally, it is necessary to compare our algorithm with the matrix-based one in cases when the size difference between Chomsky Normal Form and ECFG representation of the query is significant.

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