

Context-Free Path Querying with Single-Path Semantics by Matrix Multiplication

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ABSTRACT

A recent study showed that the applicability of context-free path querying (CFPQ) algorithms with relational query semantics integrated with Neo4j database is limited because of low performance and high memory consumption. In this work we implement a matrix-based CFPQ algorithm by using appropriate high-performance libraries for linear algebra and integrate it with RedisGraph graph database. Also, we introduce a new CFPQ algorithm with single-path query semantics that allows us to extract one found path for each pair of nodes. Finally, we provide the evaluation of our algorithms for both semantics which shows that matrix-based CFPQ implementation for RedisGraph database is performant enough for real-world data analysis.

CCS CONCEPTS

• **Information systems** → Query languages for non-relational engines; • **Theory of computation** → Grammars and context-free languages; *Parallel computing models*; • **Computing methodologies** → Massively parallel algorithms; • **Computer systems organization** → Single instruction, multiple data;

KEYWORDS

Context-free path querying, transitive closure, graph databases, RedisGraph database, linear algebra, context-free grammar, GPGPU, CUDA, Boolean matrix, matrix multiplication

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1 INTRODUCTION

Formal language constrained path querying, or formal language constrained path problem [3], is a graph analysis problem in which formal languages are used as constraints for navigational path queries. In this approach a path is viewed as a word constructed by concatenation of edge labels. Paths of interest are constrained with some formal language: a query should find only paths labeled by words from the language. The class of language constraints which is most widely spread is regular: it is used in various graph query languages and engines. Context-free path querying (CFPQ) [27], while being more expressive, is still at the early stage of development. Context-free constraints allow one to express such important class of queries as *same generation queries* [1] which cannot be expressed in terms of regular constraints.

Several algorithms for CFPQ based on such parsing techniques as (G)LL, (G)LR, and CYK were proposed recently [5, 6, 11, 13, 17, 21, 24, 26, 28]. Yet recent research by Jochem Kuijpers et.al. [16] shows that existing solutions are not applicable for real-world graph analysis because of significant running time and memory consumption. At the same time, Nikita Mishin et.al show in [19] that the matrix-based CFPQ algorithm demonstrates good performance on real-world data. A matrix-based algorithm proposed by Rustam Azimov [2] offloads the most critical computations onto Boolean matrices multiplication. This algorithm is easy to implement and to employ modern massive-parallel hardware for CFPQ. The paper measures the performance of the algorithm in isolation while J. Kuijpers provides the evaluation of the algorithms which are integrated with Neo4j¹ graph database. Also, in [16] the matrix-based algorithm is implemented as a simple single-thread Java program, while N. Mishin shows that to achieve the best performance, one should utilize high-performance matrix multiplication libraries which are

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¹Neo4j graph database web page: <https://neo4j.com/>. Access date: 12.11.2019.

highly parallel or utilize GPGPU better. Thus, it is required to evaluate a matrix-based algorithm which is integrated with a graph storage and makes use of performant libraries and hardware.

All discussed matrix-based algorithms correspond to the CFPQ with relational query semantics (according to Hellings [12]) and solve the reachability problem. However, in some cases it is important to have a proof of existence of certain paths. This problem can be solved using CFPQ algorithms with single-path query semantics (according to Hellings [13]), which provide some path for each node pair if one exists. There are many results on the CFPQ with single-path query semantics which use the shortest paths to return [3, 5, 13, 25]. We provide the algorithm for CFPQ with single-path query semantics which, for performance reasons, returns a path corresponding to the string with derivation tree of minimal height. However, our algorithm can be easily modified to return the shortest paths.

In this work, we show that CFPQ with relational and single-path query semantics can be performant enough to be applicable to real-world graph analysis. We use RedisGraph² [7] graph database as a storage. This database uses adjacency matrices as a representation of a graph and GraphBLAS [15] for matrices manipulation. These facts allow us to integrate matrix-based CFPQ algorithm with RedisGraph with minimal effort. We make the following contributions in this paper.

- (1) We provide the first matrix-based algorithm for CFPQ with single-path query semantics and prove the correctness of this algorithm.
- (2) We provide a number of implementations of the CFPQ algorithms for relational and single-path query semantics which are based on matrix multiplication and uses RedisGraph as graph storage. The first implementation for relational query semantics is CPU-based and utilizes SuteSparse³ [9] implementation of GraphBLAS API for matrices manipulation. Also, we provide GPGPU-based implementation for relational query semantics: the CUSP⁴-based implementation and the implementation based on the idea from the paper [20]. Finally, we provide the GPGPU-based implementation for the proposed CFPQ algorithm with single-path query semantics. The source code is available on GitHub⁵.
- (3) We extend the dataset presented in [19] with new real-world and synthetic cases of CFPQ⁶.
- (4) We provide evaluation which shows that matrix-based CFPQ implementation for RedisGraph database is performant enough for real-world data analysis.

²RedisGraph is a graph database which is based on Property Graph Model. Project web page: <https://oss.redislabs.com/redisgraph/>. Access date: 12.11.2019.

³SuteSparse is a sparse matrix software which includes GraphBLAS API implementation. Project web page: <http://faculty.cse.tamu.edu/davis/sutesparse.html>. Access date: 12.11.2019.

⁴CUSP is an open source library for sparse matrix multiplication on GPGPU. Project site: <https://cusplibrary.github.io/>. Access date: 12.11.2019.

⁵Sources of matrix-based CFPQ algorithm for RedisGraph database: <https://github.com/YaccConstructor/RedisGraph>. Access date: 12.11.2019.

⁶The CFPQ_Data dataset for CFPQ algorithms evaluation and comparison. GitHub page: https://github.com/JetBrains-Research/CFPQ_Data. Access date: 12.11.2019.

2 THE MOTIVATING EXAMPLE

In this section, we formulate the problem of context-free path query evaluation, using a small graph and the classical *same-generation query* [1], which cannot be expressed using regular expressions.

Let us have a graph database or any other object, which can be represented as a graph. The same-generation query can be used for discovering a vertex similarity, for example, gene similarity [22]. For graph databases, the same-generation query is aimed at the finding all the nodes at the same hierarchy level. The language, formed by the paths between such nodes, is not regular and corresponds to the language of matching parentheses. Hence, the query is formulated as a context-free grammar.

For example, let us have a small double-cyclic graph (see Figure 1). One of the cycles has three edges, labeled with *a*, and the other has two edges, labeled with *b*. Both cycles are connected via a shared node 0.

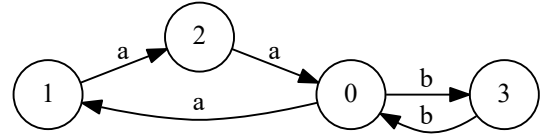


Figure 1: An example graph.

For this graph, we have a same-generation query, formulated as a context-free grammar, which generates a context-free language $L = \{a^n b^n \mid n \geq 1\}$.

The result of context-free path query evaluation w.r.t the relational query semantics for this example is a set of node pairs (m, n) , such that there is a path from the node m to the node n , whose labeling forms a word from the language L . For example, the node pair $(0, 0)$ must be in this set, since there is a path from the node 0 to the node 0, whose labeling forms a string $w = aaaaabbbbbb = a^6 b^6 \in L$.

The result of context-free path query evaluation w.r.t the single-path query semantics also contains such a path for each node pair (m, n) returned after the context-free path query evaluation w.r.t the relational query semantics. For example, a path from the node 0 to the node 0, whose labeling forms a string $w = a^6 b^6$ can be returned for the node pair $(0, 0)$.

3 PRELIMINARIES

Let Σ be a finite set of edge labels. Define an *edge-labeled directed graph* as a tuple $D = (V, E)$ with a set of nodes V and a directed edge relation $E \subseteq V \times \Sigma \times V$.

A path π is a list of labeled edges $[e_1, \dots, e_n]$ where $e_i \in E$. The concatenation of a path π_1 with a path π_2 we denote by $\pi_1 + \pi_2$.

For a path π in a graph D , we denote the unique word, obtained by concatenating the labels of the edges along the path π as $l(\pi)$. Also, we write $n\pi m$ to indicate, that the path π starts at the node $n \in V$ and ends at the node $m \in V$.

A *context-free grammar* is a triple $G = (N, \Sigma, P)$, where N is a finite set of non-terminals, Σ is a finite set of terminals, and P is a finite set of productions of the following forms:

- $A \rightarrow BC$, for $A, B, C \in N$,

- $A \rightarrow x$, for $A \in N$ and $x \in \Sigma \cup \{\varepsilon\}$.

We use the conventional notation $A \xRightarrow{*}_G w$ to denote, that a string $w \in \Sigma^*$ can be derived from a non-terminal A by some sequence of production rule applications from P in grammar G . The *language* of a grammar $G = (N, \Sigma, P)$ with respect to a start non-terminal $S \in N$ is defined by

$$L(G_S) = \{w \in \Sigma^* \mid S \xRightarrow{*}_G w\}.$$

For a given graph $D = (V, E)$ and a context-free grammar $G = (N, \Sigma, P)$, we define *context-free relations* $R_A \subseteq V \times V$ for every $A \in N$, such that

$$R_A = \{(n, m) \mid \exists n\pi m (l(\pi) \in L(G_A))\}.$$

For the context-free path query evaluation w.r.t. the single-path query semantics, we must provide such a path for each node pair from R_A . In order to do this, we introduce the

$$PathIndex = (left, right, middle, height, length)$$

— the elements of matrices which describe the found paths as concatenations of two smaller paths and help to restore each path and derivation tree for it at the end of evaluation. Here *left* and *right* stand for the indexes of starting and ending node in the founded path, *middle* — the index of intermediate node used in the concatenation of two smaller paths, *height* — the height of the derivation tree of the string corresponding to the founded path, and *length* is a length of founded path. When we do not find the path for some node pair i, j , we use the $PathIndex = \perp = (0, 0, 0, 0, 0)$.

Also, we will use the notation *proper matrix* which means that for every element of the matrix with indexes i, j it either $PathIndex = (i, j, _, _, _)$ or \perp .

For proper matrices we use a binary operation \otimes defined for PathIndexes PI_1, PI_2 which are not equal to \perp and with $PI_1.right = PI_2.left$ as

$$PI_1 \otimes PI_2 = (PI_1.left, PI_2.right, PI_1.right, \\ \max(PI_1.height, PI_2.height) + 1, \\ PI_1.length + PI_2.length).$$

If at least one of the operands is equal to \perp then $PI_1 \otimes PI_2 = \perp$.

For proper matrices we also use a binary operation \oplus defined for PathIndexes PI_1, PI_2 which are not equal to \perp with $PI_1.left = PI_2.left$ and $PI_1.right = PI_2.right$ as PI_1 if $PI_1.height \leq PI_2.height$ and PI_2 otherwise. If only one operand is equal to \perp then $PI_1 \oplus PI_2$ equal to another operand. If both operands are equal to \perp then $PI_1 \oplus PI_2 = \perp$.

Using \otimes as multiplication of PathIndexes, and \oplus as an addition, we can define a *matrix multiplication*, $a \odot b = c$, where a and b are matrices of a suitable size, that have PathIndexes as elements, as

$$c_{i,j} = \bigoplus_{k=1}^n a_{i,k} \otimes b_{k,j}.$$

Also, we use the element-wise $+$ operation on matrices a and b with the same size: $a + b = c$, where $c_{i,j} = a_{i,j} \oplus b_{i,j}$.

4 MATRIX-BASED ALGORITHM FOR CFPQ

The matrix-based algorithm for CFPQ was proposed by Rustam Azimov [2]. This algorithm can be expressed in terms of operations over Boolean matrices (see listing 1) which is an advantage for implementation.

Listing 1 Context-free path querying algorithm

```

1: function EVALCFPQ( $D = (V, E)$ ,  $G = (N, \Sigma, P)$ )
2:    $n \leftarrow |V|$ 
3:    $T \leftarrow \{T^{A_i} \mid A_i \in N, T^{A_i} \text{ is a matrix } n \times n, T^{A_i} \leftarrow \text{false}\}$ 
4:   for all  $(i, x, j) \in E, A_k \mid A_k \rightarrow x \in P$  do  $T^{A_k}_{i,j} \leftarrow \text{true}$ 
5:   for  $A_k \mid A_k \rightarrow \varepsilon \in P$  do  $T^{A_k}_{i,i} \leftarrow \text{true}$ 
6:   while any matrix in  $T$  is changing do
7:     for  $A_i \rightarrow A_j A_k \in P$  do  $T^{A_i} \leftarrow T^{A_i} + (T^{A_j} \times T^{A_k})$ 
8:   return  $T$ 

```

Here $D = (V, E)$ is the input graph and $G = (N, \Sigma, P)$ is the input grammar. For each matrix T^{A_k} indexed with a nonterminal $A_k \in N$, a cell holds a true value ($T^{A_k}_{i,j} = \text{true}$) if and only if there exists $i\pi j$ — a path in D such that $A_k \xRightarrow{*}_G l(\pi)$, where $l(\pi)$ is a word formed by the labels along the path π . Thus, this algorithm solves the reachability problem, or, according to Hellings [12], implements relational query semantics.

The performance-critical part of the algorithm is Boolean matrix multiplication, thus one can achieve better performance by using libraries which efficiently multiply boolean matrices. There is also the following optimization: if the matrices T^{A_j} and T^{A_k} have not changed at the previous iteration, then we can skip the update operation in line 7. Data in real-world problems is often sparse, thus employing libraries which manipulate sparse matrices improves running time even more.

5 MATRIX-BASED CFPQ FOR SINGLE-PATH SEMANTICS

In this section, we propose the matrix-based algorithm for CFPQ w.r.t. the single-path query semantics (see listing 2). This algorithm constructs the set of matrices T with PathIndexes as elements.

Listing 2 CFPQ algorithm w.r.t. single-path query semantics

```

1: function EVALCFPQ( $D = (V, E)$ ,  $G = (N, \Sigma, P)$ )
2:    $n \leftarrow |V|$ 
3:    $T \leftarrow \{T^{A_i} \mid A_i \in N, T^{A_i} \text{ is a matrix } n \times n, T^{A_i} \leftarrow \perp\}$ 
4:   for all  $(i, x, j) \in E, A_k \mid A_k \rightarrow x \in P$  do  $T^{A_k}_{i,j} \leftarrow (i, j, i, 1, 1)$ 
5:   for  $A_k \mid A_k \rightarrow \varepsilon \in P$  do  $T^{A_k}_{i,i} \leftarrow (i, i, i, 1, 0)$ 
6:   while any matrix in  $T$  is changing do
7:     for  $A_i \rightarrow A_j A_k \in P$  do  $T^{A_i} \leftarrow T^{A_i} + (T^{A_j} \odot T^{A_k})$ 
8:   return  $T$ 

```

After constructing the set of matrices T for every node pair i, j and nonterminal A we can extract a path $i\pi j$ from i to j such that $A \xRightarrow{*}_G l(\pi)$ if such path exists. We also propose the algorithm (see listing 3) for extracting one of those paths which forms a string with

minimal height of derivation tree. Our algorithm returns the empty path $[]$ only if $i = j$ and $A \rightarrow \varepsilon \in P$. Note that if the PathIndex for given i, j, A is equal to \perp then our algorithm returns a special path π_\emptyset to denote that such a path does not exist.

Listing 3 Path extraction algorithm

```

1: function EXTRACTPATH( $i, j, A, T = \{T^{A_i}\}, G = (N, \Sigma, P)$ )
2:    $index \leftarrow T_{i,j}^A$ 
3:   if  $index = \perp$  then
4:     return  $\pi_\emptyset$  ▷ Such a path does not exist
5:   if  $index.height = 1$  then
6:     if  $index.length = 0$  then
7:       return  $[]$  ▷ Return an empty path
8:     for all  $x \mid (i, x, j) \in E$  do
9:       if  $A \rightarrow x \in P$  then
10:        return  $[(i, x, j)]$  ▷ Return a path of length one
11:   for all  $A \rightarrow BC \in P$  do
12:      $index_B \leftarrow T_{i,index.middle}^B$ 
13:      $index_C \leftarrow T_{index.middle,j}^C$ 
14:     if  $(index_B \neq \perp) \wedge (index_C \neq \perp)$  then
15:        $maxH \leftarrow \max(index_B.height, index_C.height)$ 
16:       if  $index.height = maxH + 1$  then
17:          $\pi_1 \leftarrow \text{EXTRACTPATH}(i, index.middle, B, T, G)$ 
18:          $\pi_2 \leftarrow \text{EXTRACTPATH}(index.middle, j, C, T, G)$ 
19:       return  $\pi_1 + \pi_2$ 
    
```

5.1 Correctness

Let $T^{(p)} = \{T^{(p),A_i}\}$ be a constructed matrix T by the algorithm in listing 2 after $p - 1$ loop iterations for $p \geq 2$, and $T^{(1)} = \{T^{(1),A_i}\}$ be a constructed matrix T by this algorithm after initialization in lines 3-5. Note that the matrix T returned by this algorithm is equal to $\sum_{p=1}^\infty T^{(p)}$. Then the following lemma and theorem hold.

LEMMA 5.1. *Let $D = (V, E)$ be a graph, let $G = (N, \Sigma, P)$ be a grammar. Then for any i, j and for any non-terminal $A \in N$, $index = T_{i,j}^{(p),A}$ and $index = (i, j, k, h, l) \neq \perp$ iff $(i, j) \in R_A$ and $i\pi j$, such that there is a derivation tree of the minimal height $h \leq p$ for the string $l(\pi)$ of length l and a context-free grammar $G_A = (N, \Sigma, P, A)$.*

PROOF. (Proof by Induction)

Base case: Show that the lemma holds for $p = 1$. For any i, j and for any non-terminal $A \in N$, $(i, j, k, h, l) = T_{i,j}^{(1),A}$ iff there is either $i\pi j$ of length 1 that consists of a unique edge e from the node i to the node j and $(A \rightarrow x) \in P$, where $x = l(\pi)$, or $i = j$ and $(A \rightarrow \varepsilon) \in P$, where $\varepsilon = l(\pi)$. Therefore $(i, j) \in R_A$ and there is a derivation tree of the minimal height $h = p = 1$, shown on Figure 2, for the string x and a context-free grammar $G_A = (N, \Sigma, P, A)$. Thus, it has been shown that the lemma holds for $p = 1$.

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

The index $(i, j, k, h, l) = T_{i,j}^{(q),A}$ iff there exists a rule $(A \rightarrow BC) \in P$ such that $(i, j, k, h, l) = M_{i,j}$ where

$$M = T^{(q-1),A} + (T^{(q-1),B} \odot T^{(q-1),C}).$$

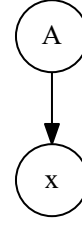


Figure 2: The derivation tree of the minimal height $p = 1$ for the string $x = l(\pi)$ where $x \in \Sigma \cup \{\varepsilon\}$.

Let $(i, j, k, h, l) = T_{i,j}^{(q-1),A}$. By the inductive hypothesis, $(i, j, k, h, l) = T_{i,j}^{(q-1),A}$ iff $(i, j) \in R_A$ and there exists $i\pi j$, such that there is a derivation tree of the minimal height $h \leq (q - 1)$ for the string $l(\pi)$ and a context-free grammar $G_A = (N, \Sigma, P, A)$. The statement of the lemma holds for $p = q$ since the height h of this tree is also less than or equal to q .

Now, let $(i, j, k, h, l) = (T^{(q-1),B} \odot T^{(q-1),C})_{i,j}$. By the definition of the binary operation \odot , $(i, j, k, h, l) = (T^{(q-1),B} \odot T^{(q-1),C})_{i,j}$ iff there are $r = k$, $(i, r, _, h_1, l_1) = T_{i,r}^{(q-1),B}$ and $(r, j, _, h_2, l_2) = T_{r,j}^{(q-1),C}$, such that $q = \max(h_1, h_2) + 1$, $l = l_1 + l_2$. Hence, by the inductive hypothesis, there are $i\pi_1 r$ and $r\pi_2 j$, such that $(i, r) \in R_B$ and $(r, j) \in R_C$, and there are the derivation trees T_B and T_C of minimal heights $h_1 \leq (q - 1)$ and $h_2 \leq (p - 1)$ for the strings $w_1 = l(\pi_1)$, $w_2 = l(\pi_2)$ and the context-free grammars G_B, G_C respectively. Thus, the concatenation of paths π_1 and π_2 is $i\pi j$, where $(i, j) \in R_A$ and there is a derivation tree of the minimal height $h = 1 + \max(h_1, h_2)$, shown on Figure 3, for the string $w = l(\pi)$ of length $l = l_1 + l_2$ and a grammar G_A .

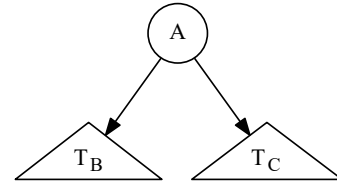


Figure 3: The derivation tree of the minimal height $h = 1 + \max(h_1, h_2)$ for the string $w = l(\pi)$, where T_B and T_C are the derivation trees for strings w_1 and w_2 respectively.

The statement of the lemma holds for $p = q$ since the minimal height $h = 1 + \max(h_1, h_2) \leq q$. This completes the proof of the lemma. \square

THEOREM 1. *Let $D = (V, E)$ be a graph and let $G = (N, \Sigma, P)$ be a grammar. Then for any i, j and for any non-terminal $A \in N$, $index = T_{i,j}^A$ and $index = (i, j, k, h, l) \neq \perp$ iff $(i, j) \in R_A$ and $i\pi j$, such that there is a derivation tree of the minimal height h for the string $l(\pi)$ of length l and a context-free grammar $G_A = (N, \Sigma, P, A)$.*

PROOF. Since the matrix $T = \sum_{p=1}^\infty T^{(p)}$ for any i, j and for any non-terminal $A \in N$, $index = T_{i,j}^A$ and $index = (i, j, k, h, l) \neq \perp$

iff there is $p \geq 1$, such that $index \in T_{i,j}^{(p),A}$. By the lemma 5.1, $index = T_{i,j}^{(p),A}$ iff $(i, j) \in R_A$ and $i\pi j$, such that there is a derivation tree of the minimal height $h \leq p$ for the string $l(\pi)$ of length l and a context-free grammar $G_A = (N, \Sigma, P, A)$. This completes the proof of the theorem. \square

Now, using the theorem 1 and induction on the length of the path, it can be easily shown that the following theorem holds.

THEOREM 2. *Let $D = (V, E)$ be a graph, let $G = (N, \Sigma, P)$ be a grammar and T be a set of matrices returned by the algorithm in listing 2. Then for any i, j and for any non-terminal $A \in N$ such that $index = T_{i,j}^A$ and $index = (i, j, k, h, l) \neq \perp$, the algorithm in listing 3 for these parameters will return a path $i\pi j$ such that $(i, j) \in R_A$ and there is a derivation tree of the minimal height h for the string $l(\pi)$ of length l and a context-free grammar $G_A = (N, \Sigma, P, A)$.*

We can, therefore, determine whether $(i, j) \in R_A$ by asking whether $T_{i,j}^A = \perp$. Also, we can extract such a path which forms a string with a derivation tree of minimal height by using our algorithm in listing 3. Thus, we show how the context-free path query evaluation w.r.t. the single-path semantics can be solved in terms of matrix operations.

5.2 Complexity

Denote the number of elementary operations executed by the algorithm of multiplying two $n \times n$ matrices with PathIndexes as $MM(n)$. Also, denote the number of elementary operations, executed by the matrix element-wise $+$ operation of two $n \times n$ matrices with PathIndexes as $MA(n)$. Since the line 7 of the algorithm in listing 2 is executed no more than $|V|^2|N|$ times, the following theorem holds.

THEOREM 3. *Let $D = (V, E)$ be a graph and let $G = (N, \Sigma, P)$ be a grammar. The algorithm in listing 2 calculates the set of matrices T in $O(|V|^2|N|^3(MM(|V|) + MA(|V|)))$.*

Also, denote the time complexity of the access to the PathIndex in the $n \times n$ matrix as $Access(n)$. Then the following theorem on the time complexity of the path extraction algorithm holds.

THEOREM 4. *Let $D = (V, E)$ be a graph, let $G = (N, \Sigma, P)$ be a grammar and T be a set of matrices returned by the algorithm in listing 2. Then for any i, j and for any non-terminal $A \in N$ such that $index = T_{i,j}^A$ and $index = (i, j, k, h, l) \neq \perp$, the algorithm in listing 3 for these parameters calculates a path $i\pi j$ in $O(l \times N \times Access(|V|))$.*

5.3 An Example

In this section, we provide a step-by-step demonstration of the proposed algorithms. For this, we consider the example with the worst-case time complexity.

The **example query** is based on the context-free grammar $G = (N, \Sigma, P)$ of the worst-case example query where:

- the set of non-terminals $N = \{S\}$;
- the set of terminals $\Sigma = \{a, b\}$;
- the set of production rules P is presented on Figure 4.

Since the proposed algorithm processes only grammars in Chomsky normal form, we first transform the grammar G into an equivalent grammar $G' = (N', \Sigma', P')$ in normal form, where:

$$\begin{aligned} 0 : S &\rightarrow a S b \\ 1 : S &\rightarrow a b \end{aligned}$$

Figure 4: Production rules for the worst-case example.

- the set of non-terminals $N' = \{S, S_1, A, B\}$;
- the set of terminals $\Sigma' = \{a, b\}$;
- the set of production rules P' is presented on Figure 5.

$$\begin{aligned} 0 : S &\rightarrow A B \\ 1 : S &\rightarrow A S_1 \\ 2 : S_1 &\rightarrow S B \\ 3 : A &\rightarrow a \\ 4 : B &\rightarrow b \end{aligned}$$

Figure 5: Production rules for the example query grammar in normal form.

We run the query on a graph, presented on Figure 1. We provide a step-by-step demonstration of the work with the given graph D and grammar G' of the algorithm in listing 2. After the matrix initialization in lines 3-5 of this algorithm, we have a matrix $T^{(1)}$, presented on Figure 6.

$$\begin{aligned} T^{(1),A} &= \begin{pmatrix} \perp & (0, 1, 0, 1, 1) & \perp & \perp \\ \perp & \perp & (1, 2, 1, 1, 1) & \perp \\ (2, 0, 2, 1, 1) & \perp & \perp & \perp \\ \perp & \perp & \perp & \perp \end{pmatrix} \\ T^{(1),B} &= \begin{pmatrix} \perp & \{A\} & \perp & (0, 3, 0, 1, 1) \\ \perp & \perp & \{A\} & \perp \\ \{A\} & \perp & \perp & \perp \\ (3, 0, 3, 1, 1) & \perp & \perp & \perp \end{pmatrix} \end{aligned}$$

Figure 6: The initial matrix for the example query. The PathIndexes $T_{i,j}^{(1),S_1}$ and $T_{i,j}^{(1),S}$ are equal to \perp for every i, j .

After the initialization the only matrices which will be updated are T^{S_1} and T^S . These matrices obtained after first loop iteration is shown on Figure 7.

$$T^{(2),S} = \begin{pmatrix} \perp & \perp & \perp & \perp \\ \perp & \perp & \perp & \perp \\ \perp & \perp & \perp & (2, 3, 0, 2, 2) \\ \perp & \perp & \perp & \perp \end{pmatrix}$$

Figure 7: The first iteration of computing the transitive closure for the example query. The PathIndexes $T_{i,j}^{(1),S_1}$ are equal to \perp for every i, j .

When the algorithm at some iteration finds new paths for some nonterminal in the graph D , then it adds corresponding PathIndexes

to the matrix for this nonterminal. For example, after the first loop iteration, PathIndex (2, 3, 0, 2, 2) is added to the matrix T^S . This PathIndex is added to the element with a row index $i = 2$ and a column index $j = 3$. This means, that there is $i\pi j$ (a path π from the node 2 to the node 3), such that $S \xrightarrow[G]{*} l(\pi)$, this path obtained by concatenation of smaller paths via node 0, the length of path is equal to 2, and the derivation tree for the string $l(\pi)$ has a height 2.

The calculation of the transitive closure is completed after k iterations, when a fixpoint is reached: $T^{(k)} = T^{(k+1)}$. For the example query, $k = 13$ since $T_{13} = T_{14}$. The resulted matrices are presented on Figure 8.

$$T^{(14),S} = \begin{pmatrix} (0, 0, 1, 12, 12) & \perp & \perp & (0, 3, 1, 6, 6) \\ (1, 0, 2, 4, 4) & \perp & \perp & (1, 3, 2, 10, 10) \\ (2, 0, 0, 8, 8) & \perp & \perp & (2, 3, 0, 2, 2) \\ \perp & \perp & \perp & \perp \end{pmatrix}$$

$$T^{(14),S_1} = \begin{pmatrix} (0, 0, 3, 7, 7) & \perp & \perp & (0, 3, 0, 13, 13) \\ (1, 0, 3, 11, 11) & \perp & \perp & (1, 3, 0, 5, 5) \\ (2, 0, 3, 3, 3) & \perp & \perp & (2, 3, 0, 9, 9) \\ \perp & \perp & \perp & \perp \end{pmatrix}$$

Figure 8: The final matrices after computing the transitive closure for the example query.

Thus, the result of the algorithm in listing 2 for the example query are the matrices on Figures 6 and 8. Now, after constructing the transitive closure, we can construct the context-free relations R_A . These relations for each non-terminal of the grammar G' are presented on Figure 9.

$$\begin{aligned} R_S &= \{(0, 0), (0, 3), (1, 0), (1, 3), (2, 0), (2, 3)\}, \\ R_{S_1} &= \{(0, 0), (0, 3), (1, 0), (1, 3), (2, 0), (2, 3)\}, \\ R_A &= \{(0, 1), (1, 2), (2, 0)\}, \\ R_B &= \{(0, 3), (3, 0)\}. \end{aligned}$$

Figure 9: Context-free relations for the example query.

In the context-free relation R_S , we have all node pairs corresponding to paths, whose labeling is in the language $L(G_S) = \{a^n b^n | n \geq 1\}$. Using the algorithm in listing 3 we can restore paths for each node pair from context-free relations. For example, given $i = j = 0$, nonterminal S , set of resulted matrices T , and context-free grammar G' , the algorithm in listing 3 returns a path $0\pi 0$ whose labeling forms a string $l(\pi) = a^6 b^6$. The length of path π is equal to 12 and the height of the derivation tree for $l(\pi)$ is equal to 12, which is consistent with the corresponding PathIndex $T_{0,0}^{(14),S}$.

6 IMPLEMENTATION DETAILS

We showed that CFPQ can be naturally reduced to linear algebra. Linear algebra for graph problems is an actively developed area. One of the most important results is a GraphBLAS API which

provides a way to operate over matrices and vectors over user-defined semirings.

Previous works show [2, 19] that existing linear algebra libraries utilization is the right way to achieve high-performance CFPQ implementation with minimal effort. But neither of these works provide an evaluation with data storage: algorithm execution time has been measured in isolation.

We provide a number of implementations of the matrix-based CFPQ algorithm. We use RedisGraph as storage and implement CFPQ as an extension by using the mechanism provided. Note that currently, we do not provide complete integration with the querying mechanism: one cannot use Cypher — a query language used in RedisGraph. Instead, a query should be provided explicitly as a file with grammar in Chomsky normal form. This is enough to evaluate querying algorithms and we plan to improve integration in the future to make our solution easier to use.

Below we show an index building algorithm for extracting paths using both the GPU and the CPU. The **path extraction** algorithm currently has only the CPU version. This is a conscious choice because the current path extraction algorithm does not adapt well to the GPGPU architecture (it is difficult to create coalesced access to global memory during executing of the algorithm for multiple vertices).

Both **CPU-based implementation** use SuiteSparse implementation of GraphBLAS, which is also used in RedisGraph and provides a set of sparse matrix operation.

The first one (**RG_CPU_{rel}**) implements relational path semantics problem. It utilizes RedisGraph relationship adjacency matrices, so we avoid data format issues. For addition and multiplication of matrices we use the standard Boolean semiring provided by SuiteSparse.

The second (**RG_CPU_{path}**) solves the problem for the single-path query semantics. SuiteSparse supports creation of custom semiring, so we implemented all the operations over *PathIndex* in a simple way thanks to GraphBLAS API.

GPGPU-based implementation has three versions. The first one (**RG_CUSP_{rel}**) utilizes a CUSP [8] library for matrix operations, the second one (**RG_SPARSE_{rel}**) is our implementation based on the idea from paper [20] and the third one (**RG_SPARSE_{path}**) is our implementation for the single-path query semantics. First implementation require matrix format conversion but the last two do not.

We choose the CUSP library as base solution which uses sparse matrices because dense matrices cannot be applied to huge graphs. CUSP is a C++ templated library which allows us to multiply Boolean matrices (that solves relational path semantics problem). But in fact, performing CFPQ with relational paths semantics on the largest graph using CUSP does not fit in GPU memory and this fact led us to develop an algorithm that would be more memory efficient.

The second (**RG_SPARSE_{rel}**) implementation utilizes low-latency on-chip shared memory for hash table of each row of the result matrix. For more details of algorithm see the original paper [20]. An original solution designed for single and double precision SpGEMM. Since we have a Boolean matrix in CSR format, we can discard the array of values and optimize usage of shared memory. But Boolean matrix multiplication is only one part of the algorithm, since we

must effectively combine two Boolean sparse matrices. We use merge path [10] algorithm to merge corresponding rows of the result matrix.

The third (**RG_SPARSE_{path}**) algorithm must perform matrix multiplication and addition over *PathIndex* semiring. To solve this problem, we must answer three following questions.

- How to determine the size and structure of final sparse matrices?
- How to map tasks with variable complexity to the GPU?
- How to accumulate intermediate result of multiplication?

The first problem is how to determine the size and structure of final sparse matrices. Since we have the **RG_SPARSE_{rel}** algorithm we naturally know the final size and structure of all sparse matrices. Therefore we run the **RG_SPARSE_{rel}** algorithm on first step.

The second problem is how to map tasks with variable complexity to the GPU. Assume that we must to calculate $C = C + (A * B)$ multiple times. The final structure of the matrix C already known, so we can fill it with the \perp values before starting. We assign each row of the matrix C to one CUDA block. Since we know how many values exist in each row, our algorithm divides the rows into groups and applies the same configuration parameters (shared memory size, block size) for each row from one group.

The third problem is how to accumulate intermediate result of multiplication. Since we already know final structure of matrices we can accumulate results without additionally memory allocations. But for make it possible we must learn how to perform atomically \oplus operation defined for *PathIndex*. For every element of the matrix with indexes i, j it either $PathIndex = (i, j, _, _)$ or \perp . Also note that *length* information does not matter in the algorithm and can be restored later, so only two elements are really important: *middle* and *height*. We can store two 4 bytes value into one 8 byte value and perform an atomic operation. In high four bytes we store the *height* and in the low four bytes we store the *middle*. For the value of \perp we use maximum unsigned integer value of 8 bytes in size. Now we can use *atomicMin* as \oplus .

7 EVALUATION AND DISCUSSION

We evaluate all the described implementations on real-world RDFs. We measure the full time of query execution including all overhead on data preparation. This way we can estimate the applicability of the matrix-based algorithm to real-world problems.

For evaluation, we use a PC with Ubuntu 18.04 installed. It has Intel core i7-6700 CPU, 3.4GHz, DDR4 32Gb RAM, and Geforce GTX 1070 GPGPU with 8Gb RAM.

7.1 Dataset

As far as it was shown that matrix-based CFPQ algorithms are performant enough to handle big RDF [19], we extend CFPQ_Data dataset [19] with new RDFs: *go-hierarchy*, *go*, *enzyme*, *core*, *pathways*, *eclass-514en*, and use the extended dataset in our evaluation. Also we add Geospecies RDF and related query from [16]. Detailed description of the dataset and queries are provided in appendix A.

7.2 Evaluation Results

We provide results only for a part of the collected dataset because of the page limit. Running time is measured in seconds, RAM memory consumption is measured in megabytes unless specified otherwise.

The results of the CFPQ evaluation are presented in tables 1, ?? and 2. We can see that the running time of both CPU and GPGPU versions for the relational query semantics is small even for graphs with a big number of vertices and edges. The relatively small number of edges of interest may be the reason for such behavior. We believe it is necessary to extend the dataset with new queries which involve more different types of edges. Also, we can see, that **RG_CUSP_{rel}** implementation which uses dense bit matrices requires more memory. Thus we recommend to use sparse matrices on GPGPU.

As we can see, the matrix-based algorithm for relational query semantics implemented for RedisGraph is more than 1000 times faster than the one based on annotated grammar implemented for Neo4j [16] and uses more than 4 times less memory. We can conclude that the matrix-based algorithm is more performant than other CFPQ algorithms for query evaluation under a relational semantics for real-world data processing.

Also, we can see, that the GPGPU version which utilizes sparse matrices is significantly faster than the other implementations especially on big graphs. For example, for Geospaces it more than 7 times faster in both relational and single-path scenarios. Note, that for GPGPU versions we include time required for data transferring and formats conversion.

We can conclude, that the cost of computing matrices with *PathIndexes* for single-path query semantics is not high. On average, it is about 2 times slower than the reachability matrix calculation. The additional running time of the path extraction is presented in figure 10. As we can see, this time is small and linear in length of the path.

Finally, we conclude that the matrix-based algorithm paired with a suitable database and employing appropriate libraries for linear algebra is a promising way to make CFPQ with relational and single-path query semantics applicable for real-world data analysis. We show that SuiteSparse-based CPU implementation is performant enough to be comparable with GPGPU-based implementations on real-world data.

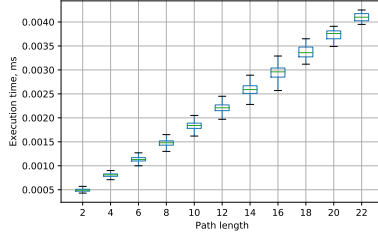
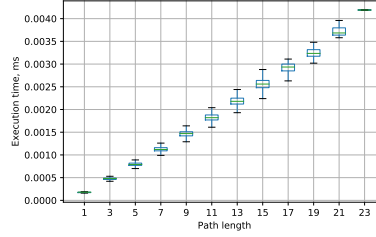
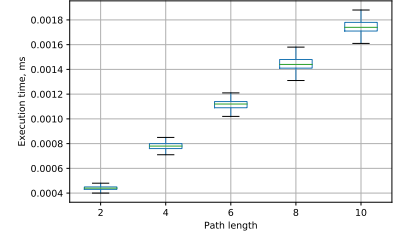
8 CONCLUSION AND FUTURE WORK

In this work, we provide the first matrix-based algorithm for CFPQ with single-path query semantics. Also, we implemented a CPU and GPGPU based CFPQ for RedisGraph and showed that CFPQ with relational and single-path query semantics can be performant enough to analyze real-world data. However, our implementations are prototypes and we plan to provide full integration of CFPQ to RedisGraph. First of all, it is necessary to extend Cypher graph query language used in RedisGraph to support syntax for specification of context-free constraints. There is a proposal which describes such syntax extension⁷. It is shown that context-free constraints can be

⁷Proposal with path pattern syntax for openCypher: <https://github.com/thobe/openCypher/blob/rpq/cip/1.accepted/CIP2017-02-06-Path-Patterns.adoc>. Access date: 12.11.2019

Table 1: RDFs query G_1

Name	Relational semantics index						Single path semantics index			
	RG_CPU _{rel}		RG_CUSP _{rel}		RG_SPARSE _{rel}		RG_CPU _{path}		RG_SPARSE _{path}	
	Time	Mem	Time	Mem	Time	Mem	Time	Mem	Time	Mem
atom-primitive	0.016	1.2	0.016	0.1	0.005	0.1	0.033	1.5	0.008	0.1
biomedical-mesure-primitive	0.016	0.6	0.012	0.1	0.005	0.1	0.027	1.3	0.007	0.1
core	0.004	0.3	0.022	2	0.01	0.1	0.002	0.3	0.016	0.1
eclass_514en	0.067	13.8	0.075	14	0.166	16	0.195	31.2	0.496	26
enzyme	0.018	5.9	0.021	0.1	0.018	4	0.029	8.1	0.043	6
foaf	0.002	0.4	0.013	0.1	0.006	0.1	0.024	0.4	0.009	0.1
funding	0.006	0.5	0.019	0.1	0.006	0.1	0.057	0.5	0.009	0.1
generations	0.002	0.3	0.01	0.1	0.004	0.1	0.013	0.3	0.005	0.1
go-hierarchy	0.091	16.3	0.433	650	0.108	121.2	0.976	92	0.336	125
go	0.604	28.8	0.59	70	0.365	30.2	1.286	75.7	0.739	45.4
pathways	0.011	0.1	0.019	0.1	0.007	0.1	0.021	0.5	0.021	2
people_pets	0.017	0.4	0.025	0.1	0.007	0.1	0.031	0.6	0.011	0.1
pizza	0.03	1.8	0.021	4	0.006	0.1	0.075	5.5	0.009	0.1
skos	0.001	0.1	0.008	0.1	0.004	0.1	0.005	0.3	0.006	0.1
travel	0.004	0.3	0.022	2	0.007	0.1	0.008	0.3	0.01	0.1
univ-bench	0.002	0.3	0.01	0.1	0.005	0.1	0.013	0.3	0.007	0.1
wine	0.017	3.5	0.032	6	0.009	0.1	0.117	7.1	0.015	0.2

(a) *go* and G_1 (b) *go* and G_2 (c) *geospices* and *geo***Figure 10: Execution time of the path extraction algorithm depending on the path length****Table 2: Geospecies querying results**

Relational semantics index				Single path semantics index			
RG_CPU _{rel}		RG_SPARSE _{rel}		RG_CPU _{path}		RG_SPARSE _{path}	
Time	Mem	Time	Mem	Time	Mem	Time	Mem
7.146	16934.2	0.856	5274	15.134	35803.6	1.935	5282

expressed with the proposed syntax and we plan to support this syntax in libcypher-parser⁸ used in RedisGraph.

The best our current GPU-based implementations (RG_SPARSE_{rel} and RG_SPARSE_{path}) have shown that it makes sense to use a GPU to speed up CFPQ on real world data. But amount of the GPU RAM usually less than the CPU RAM so one of the direction of future research is a solution that uses systems with multiple GPU.

Our implementations compute relational or single-path semantics of a query, but some problems require to find all paths which satisfies the constraints. To the best of our knowledge, there is no

matrix-based algorithm for all-path query semantics, thus we see it as a direction for future research.

Another important open question is how to update the query results dynamically when data changes. The mechanism for result updating allows one to recalculate query faster and use the result as an index for other queries. There is a theoretical results in this area [4], but they should be evaluates in practice.

Also, further improvements of the dataset are required. For example, it is necessary to include real-world cases from the area of static code analysis [14, 23, 29]. Another direction is to find new applications required CFPQ, such as for example, graph segmentation [18].

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A DATASET DESCRIPTION

In our evaluation we use dataset which contains the following parts.

Table 3: RDFs properties

Name	#V	#E	#type	#subClassOf
atom-primitive	291	685	138	122
univ-bench	179	413	84	36
travel	131	397	90	30
skos	144	323	70	1
people_pets	337	834	161	33
generations	129	351	78	0
foaf	256	815	174	10
biomed-mesure-prim	341	711	130	122
funding	778	1480	304	90
pizza	671	2604	365	259
wine	733	2450	485	126
core	1323	8684	1412	178
pathways	6238	37196	3118	3117
go-hierarchy	45007	1960436	0	490109
enzyme	48815	219390	14989	8163
eclass_514en	239111	1047454	72517	90962
go	272770	1068622	58483	90512

- The real-world data RDFs provided in CFPQ_Data dataset⁹ from [19].
- Geospecies (RDF which contains information about biological hierarchy¹⁰ and same generation query over *broadier-Transitive* relation) is provided in [16] and integrated in our evaluation with CFPQ_Data.

⁹CFPQ_Data dataset GitHub repository: https://github.com/JetBrains-Research/CFPQ_Data. Access date: 12.11.2019.

¹⁰The Geospecies RDF: <https://old.datahub.io/dataset/geospecies>. Access date: 12.11.2019.

- It was shown in [19] that matrix-based algorithm is performant enough to handle bigger RDFs than those used in the initial datasets, such as [28]. So, we add a number of big RDFs to CFPQ_Data and use them in our evaluation. New RDFs: *go-hierarchy*, *go*, *enzyme*, *core*, *pathways* are from UniProt database¹¹, and *eclass-514en* is from eClassOWL project¹².

The properties of the RDFs from the dataset are given in table 3. Geospecies RDF contains 450609 vertices, 2311461 edges, and 20867 edges labeled by *broaderTransitive*. Note that while the number of edges labeled by *broaderTransitive* is equal to provided in [16], the total number of vertices and edges is bigger. It is because we naively convert each triple from RDF to edge in the graph, while J. Kuijpers et al use special *neosemantics*¹³ plugin which can, for example, handling multivalued properties accurately.

The variants of the *same generation query* [1] are used in almost all cases because it is an important example of real-world queries that are context-free but not regular. So, variations of the same generation query are used in our evaluation. All queries are added to the CFPQ_Data dataset.

We use two queries over *subClassOf* and *type* relations. The first query is the grammar G_1 :

$$\begin{aligned} s &\rightarrow \text{subClassOf}^{-1} s \text{ subClassOf} & s &\rightarrow \text{type}^{-1} s \text{ type} \\ s &\rightarrow \text{subClassOf}^{-1} \text{subClassOf} & s &\rightarrow \text{type}^{-1} \text{type} \end{aligned}$$

The second one is the grammar G_2 :

$$s \rightarrow \text{subClassOf}^{-1} s \text{ subClassOf} \mid \text{subClassOf}$$

For geospecies we use same-generation query *geo* from the original paper [16]:

$$\begin{aligned} s &\rightarrow \text{broaderTransitive} s \text{ broaderTransitive}^{-1} \\ s &\rightarrow \text{broaderTransitive} \text{broaderTransitive}^{-1} \end{aligned}$$

B EVALUATION DETAILS

Results for RDFs querying with G_2 grammar are presented in table ??.

¹¹Protein sequences data base: <https://www.uniprot.org/>. RDFs with data are available here: ftp://ftp.uniprot.org/pub/databases/uniprot/current_release/rdf. Access date: 12.11.2019

¹²eClassOWL project: <http://www.heppnetz.de/projects/eclassowl/>. eclass-514en file is available here: http://www.ebusiness-unibw.org/ontologies/eclass/5.1.4/eclass_514en.owl. Access date: 12.11.2019.

¹³Neosemantix is an RDF processing plugin for Neo4j. Web page: <https://neo4j.com/labs/nsmtx-rdf/>. Access date: 30.03.2020.

Table 4: RDFs query G_2

Name	Relational semantics index						Single path semantics index			
	RG_CPU _{rel}		RG_CUSP _{rel}		RG_SPARSE _{rel}		RG_CPU _{path}		RG_SPARSE _{path}	
	Time	Mem	Time	Mem	Time	Mem	Time	Mem	Time	Mem
atom-primitive	0.001	0.3	0.001	0.1	0.002	0.1	0.001	0.3	0.002	0.1
biomedical-mesure-primitive	0.002	0.1	0.022	2	0.009	0.1	0.006	0.1	0.012	0.1
core	0.001	0.3	0.006	0.1	0.004	0.1	0.003	0.3	0.005	0.1
eclass_514en	0.035	6.5	0.339	16	0.1	12	0.123	17.7	0.127	18
enzyme	0.006	3.9	0.076	0.6	0.01	0.1	0.012	5.3	0.008	0.4
foaf	0.001	0.1	0.004	0.1	0.002	0.1	0.001	0.1	0.003	0.1
funding	0.002	0.1	0.015	0.4	0.007	0.1	0.009	0.1	0.008	0.1
generations	0.001	0.1	0.001	0.1	0.001	0.1	0.001	0.1	0.001	0.1
go-hierarchy	0.095	17.8	2.025	528	0.175	130.4	0.884	88.8	0.306	138.8
go	0.306	25.8	0.633	84	0.181	25.4	0.918	78.1	0.219	34.2
pathways	0.005	0.2	0.016	0.4	0.004	0.1	0.017	0.5	0.003	0.1
people_pets	0.001	0.1	0.007	0.1	0.004	0.1	0.001	0.1	0.005	0.1
pizza	0.002	0.3	0.012	0.2	0.008	0.1	0.01	0.3	0.009	0.1
skos	0.001	0.1	0.001	0.1	0.001	0.1	0.001	0.1	0.002	0.1
travel	0.001	0.1	0.007	0.1	0.005	0.1	0.001	0.1	0.005	0.1
univ-bench	0.001	0.1	0.007	0.1	0.005	0.1	0.001	0.1	0.005	0.1
wine	0.001	0.3	0.006	0.1	0.004	0.1	0.002	0.3	0.004	0.1