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

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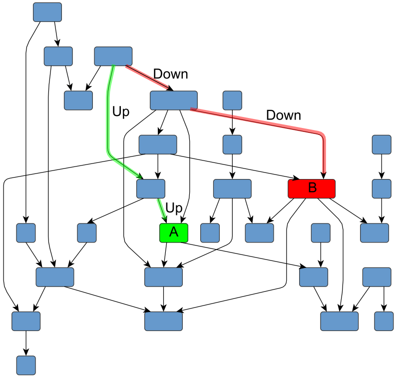
Context-Free Path Querying



Navigation through a graph

- Are nodes A and B on the same level of hierarchy?
- Is there a path of form **Up**^{n} **Down**^{n}?
- Find all paths of form **Up**^{n} **Down**^{n} which start from the node A

Context-Free Path Querying: Relational Query Semantics

- $\mathbb{G} = (\Sigma, N, P)$ — context-free grammar in normal form
  - $A \to BC$, where $A, B, C \in N$
  - $A \to x$, where $A \in N, x \in \Sigma \cup \{\varepsilon\}$
  - $L(\mathbb{G}, A) = \{\omega \mid A \Rightarrow^* \omega\}$

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  - $v \xrightarrow{l} u \in E$
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- $\omega(\pi) = \omega(v_0 \xrightarrow{l_0} v_1 \xrightarrow{l_1} \cdots \xrightarrow{l_{n-2}} v_{n-1} \xrightarrow{l_{n-1}} v_n) = l_0 l_1 \cdots l_{n-1}$

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- $R_A = \{(n, m) \mid \exists n \pi m$, such that $\omega(\pi) \in L(\mathbb{G}, A)\}$

Matrix-Based Algorithm: Relational Query Semantics

Algorithm Context-free path querying algorithm

function $\textsc{eval}\mathrm{CFPQ}(D = (V, E, L), G = (\Sigma, N, P))$
    $n \leftarrow |\mathrm{V}|$
    $T \leftarrow \{T^{A_i} \mid A_i \in N,\ T^{A_i}$ is a matrix $n \times n,\ T^{A_i}_{k,l} \leftarrow \texttt{false}\}$
    for all $(i, x, j) \in E,\ A_k \mid A_k \to x \in P$ **do** $T^{A_k}_{i,j} \leftarrow \texttt{true}$
    for all $A_k \mid A_k \to \varepsilon \in P$ **do**
        for all $i \in \{0, \ldots, n-1\}$ **do** $T^{A_k}_{i,i} \leftarrow \texttt{true}$
    while any matrix in T is changing **do**
        for $A_i \to A_j A_k \in P$ **do** $T^{A_i} \leftarrow T^{A_i} + (T^{A_j} \times T^{A_k})$
    return T

Context-Free Path Querying: Single-Path Query Semantics

- $R_A = \{(n, m) \mid \exists n\pi m$, such that $\omega(\pi) \in L(\mathbb{G}, A)\}$ — answers for the relational query semantics

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- The main idea for the matrix-based algorithm is to store additional information in adjacency matrices to be able to restore one such path $n\pi m$ for all $(n, m) \in R_A$
  - the intermediate vertex
  - some additional information about path such as length

Context-Free Path Querying: All-Path Query Semantics

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- For all $A \in N$, for all $(n, m) \in R_A$ also return **all** such paths $n\pi m$
    - the number of such paths can be infinite if the input graph has cycles
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  - usually the result is represented in the form of a finite structure such as annotated grammar or a parse forest
- Currently, our matrix-based algorithms cannot handle the all-path query semantics
- The only linear algebra-based algorithm that solves this problem is the Kronecker product-based CFPQ algorithm

Kronecker product-based algorithm

- Does not require transformation of the input grammar
- Uses Recursive State Machines for the context-free grammar representation

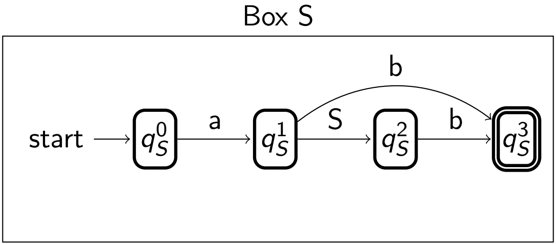

Figure: The RSM for the grammar $S \to aSb \mid ab$ of the same-generation query

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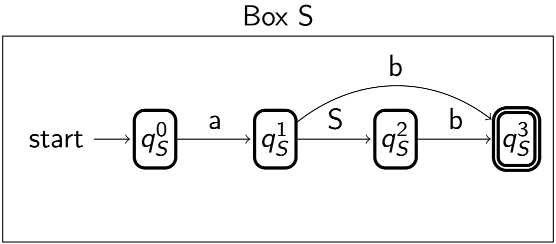


Figure: The RSM for the grammar $S \to aSb \mid ab$ of the same-generation query

- The algorithm computes the Kronecker product of the adjacency matrices of the graph for RSM and the input graph

$$\begin{pmatrix} . & \{a\} & . & . \\ . & . & \{S\} & \{b\} \\ . & . & . & \{b\} \\ . & . & . & . \end{pmatrix} \otimes \begin{pmatrix} . & \{a\} & . & . \\ . & . & \{a\} & . \\ \{a\} & . & . & \{b\} \\ . & . & \{b\} & . \end{pmatrix} =$$

$$\begin{array}{cc}
 & \begin{array}{cccc|cccc|cccc|cccc} (0,0)&(0,1)&(0,2)&(0,3)&(1,0)&(1,1)&(1,2)&(1,3)&(2,0)&(2,1)&(2,2)&(2,3)&(3,0)&(3,1)&(3,2)&(3,3) \end{array} \\
\begin{array}{c} (0,0)\\(0,1)\\(0,2)\\(0,3)\\(1,0)\\(1,1)\\(1,2)\\(1,3)\\(2,0)\\(2,1)\\(2,2)\\(2,3)\\(2,0)\\(2,1)\\(2,2)\\(2,3) \end{array} &
\left(\begin{array}{cccc|cccc|cccc|cccc}
. & . & . & . & . & \{a\} & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & \mathbf{\{a\}} & . & . & . & . & . & . & . & . & . \\
. & . & . & . & \{a\} & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
\hline
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & \mathbf{\{b\}} \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & \{b\} & . \\
\hline
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & \{b\} \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & \{b\} & . \\
\hline
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & . \\
. & . & . & . & . & . & . & . & . & . & . & . & . & . & . & .
\end{array}\right)
\end{array}$$

Research Questions

- Can we extend the matrix-based CFPQ algorithm to all-path query semantics?
- What the cost of such extension?
- How does the matrix-based solution for the all-path query semantics compare to the Kronecker product-based?

All-Path Index

- We store the additional information about the paths found as the sets of the intermediate vertices
- We introduce the following matrix multiplication operation
- $T^A \odot T^B = T^C$ where $T^C_{i,j} = \bigcup_{k=1}^{n}(T^A_{i,k} \otimes T^B_{k,j})$ and

$$T^A_{i,k} \otimes T^B_{k,j} = \begin{cases} \{k\}, & \text{if } T^A_{i,k} \neq \emptyset \wedge T^B_{k,j} \neq \emptyset \\ \emptyset, & \text{otherwise} \end{cases}$$

Matrix-Based Algorithm: All-Path Query Semantics

Algorithm CFPQ algorithm w.r.t. all-path query semantics

function $\textsc{AllPathCFPQ}($
$D = (V, E, \Sigma),$
$G = (N, \Sigma, P, S))$
  $n \leftarrow |\mathrm{V}|$
  $T \leftarrow \{ T^A \mid A \in N, T^A$ is a matrix $n \times n$, $T^A_{i,j} \leftarrow \emptyset \}$
  for all $(i, x, j) \in E$, $A \mid A \to x \in P$ **do** $T^A_{i,j} \leftarrow \{n\}$
  for all $A \mid A \to \varepsilon \in P$ **do** $T^A_{i,i} \leftarrow \{n\}$
  while any matrix in T is changing **do**
    for all $A \to BC \in P$ where T^B or T^C are changed **do**
      $T^A \leftarrow T^A + (T^B \odot T^C)$
  return T

Path extraction

- After constructing a set of matrices with sets of intermediate vertices, we can extract all required paths $i\pi j$ for every vertex pair i, j if such paths exist
- It is assumed that the sets of paths are computed lazily, to ensure the termination in case of an infinite number of paths

Implementation

- For evaluation we use the following CPU-based implementations of CFPQ algorithms with sparse matrix representation
  - *MtxRel* — for relational query semantics that uses **pygraphblas** — a Python wrapper around the GraphBLAS API
  - *MtxSingle* — for single-path query semantics that also uses **pygraphblas**
  - *MtxAll* — the implementation of the proposed matrix-based algorithm for all-path query semantics which utilizes **SuiteSparse** and our own Python wrapper
  - *Tns* — our Python implementation of the Kronecker product-based algorithm for all-path query semantics

Evaluation

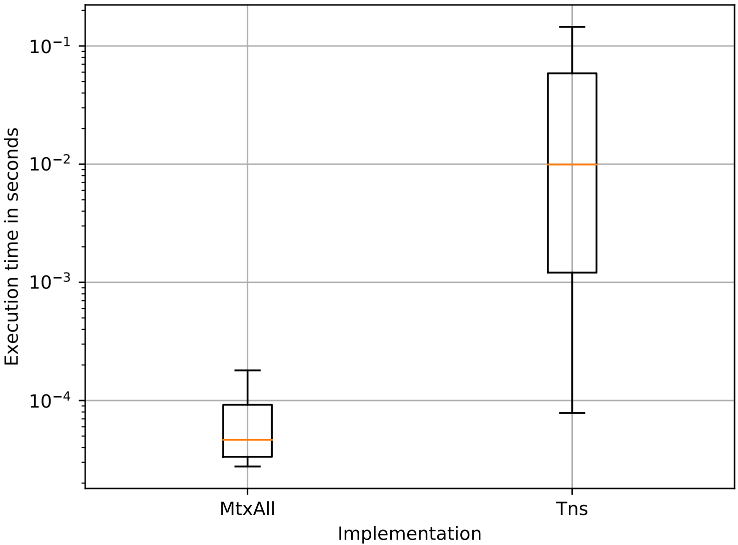
- OS: Ubuntu 18.04
- CPU: Intel core i7 6700 3,4GHz
- RAM: DDR4 64 Gb

Evaluation: CFPQ[1]

Graph	#V	#E	MtxRel		MtxSingle		MtxAll		Tns	
			Time	Mem	Time	Mem	Time	Mem	Time	Mem
pathways	6 238	18 598	0.01	140	0.01	671	0.01	49	0.01	122
go-hierarchy	45 007	980 218	0.09	255	0.84	671	0.35	195	0.24	252
enzyme	48 815	109 695	0.01	181	0.01	217	0.02	61	0.02	132
eclass_514en	239 111	523 727	0.06	181	0.16	216	0.22	126	0.27	193
go	272 770	534 311	0.94	246	0.93	217	1.13	990	1.27	243
geospecies	450 609	2 311 461	7.48	7645	15.54	22941	32.06	44235	26.32	19537
taxonomy	5 728 398	14 922 125	0.72	1175	1.15	2250	3.84	1507	3.56	1776

[1] Time in seconds and memory is measured in megabytes

Evaluation: Average Path Extraction Time For *go*



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Conclusion

- We propose a matrix-based CFPQ algorithm for all-path query semantics
- The proposed algorithm constructs index up to 2-3 times slower and consumes more memory than the algorithm for single-path query semantics
- If it is necessary to frequently recalculate the index for a changing graph or a path query then the best choice is the Kronecker product-based algorithm with faster and less memory consuming index construction
- If it is necessary to extract paths many times for a once constructed index or index changes can be efficiently computed dynamically then the proposed matrix-based CFPQ algorithm is preferable

Future Research

- We compare the CPU-based implementation. In the future, we want to obtain GPU-based and distributed implementations
- Also, further improvements in index creation and path extraction for both matrix-based and Kronecker product-based algorithms are required
- We plan to provide the multiple-source modifications for all linear algebra-based CFPQ algorithms

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- Ilya Epelbaum: iliyepelbaun@gmail.com

- Dataset: https://github.com/JetBrains-Research/CFPQ_Data
- Algorithm implementations: https://github.com/JetBrains-Research/CFPQ_PyAlgo

Thanks!