

Graph Parsing Application for Bioinformatics Problems

An affordable PXI-based microwave non-linear characterization platform

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Motivation

Biomedical databases contain huge amounts of rich data which can be represented as a labelled graph. In order to investigate such data, it may be useful to extract connections with specific constraints. One natural way to provide constraints is to specify the language of paths labels which can be done by using of grammars. For example, one can use context-free grammars with productions $\{S \rightarrow aSb; S \rightarrow \varepsilon\}$ to query paths which labels should take form of $ab; aabb; aaabbb; \dots$, or, generally, should belong to the language $L = \{a^n b^n, n \geq 0\}$. This approach is named *context-free path querying* and can be applied to some problems in bioinformatics.

Tasks described above can be solved by using common technique named graph parsing — application of classical parsing techniques for graphs; and we have some experience in this field [1, 2].

Results

Our results solve some problems of existing approaches (such as cycles processing problem in [3]), and provide an ability to use GPGPU and multi-core systems for graph parsing which can be useful for huge biological data analysis.

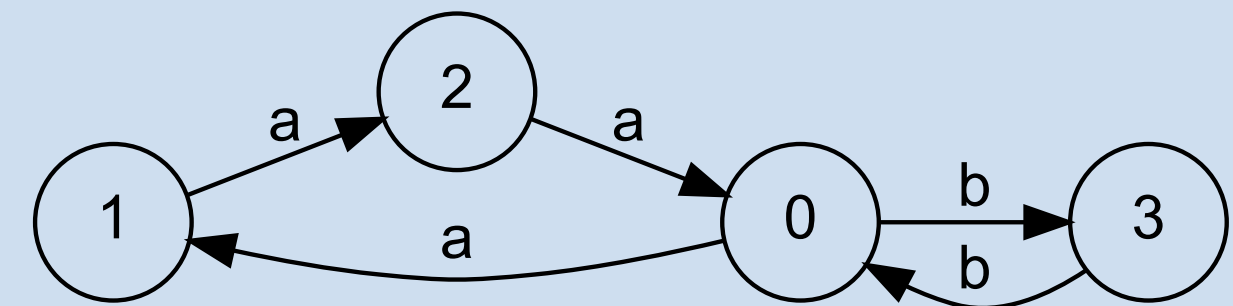
- Graph parsing framework
- !!!
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Future Research

- Currently we are working on long subsequences of 16s rRNA reconstruction from metagenomic assembly and on entities connections detection.
- Our aim is to present current results and also to find other applications for this techniques.
- Context-free compressed data processing

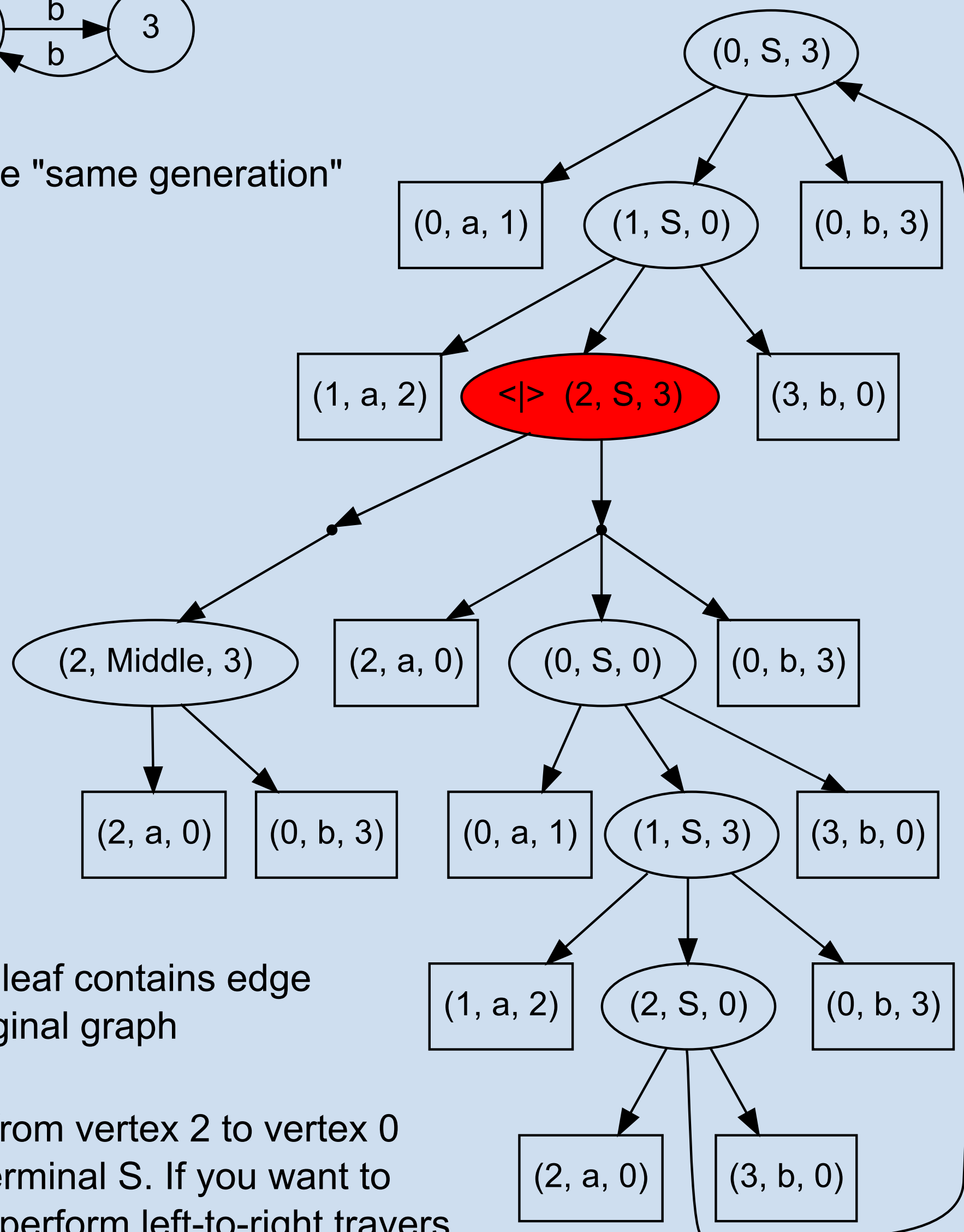
Context-free path querying

Graph-structured data



Query result: compressed parsing forest for all matched paths. Paths can be extracted by forest traversal.

Context-free grammar for the "same generation" query with marked middle:
 $S \rightarrow a S b$
 $S \rightarrow \text{Middle}$
 $\text{Middle} \rightarrow a b$



Each leaf contains edge of original graph

There exists path from vertex 2 to vertex 0 derived from nonterminal S. If you want to get this path, then perform left-to-right travers from this vertex

Possible application

One of the examples is an analysis of graphs where vertices correspond to entities and concepts such as gene or phenotype while edges represent known relationships such as “codes for”, “interacts with”, etc (UniProt dataset [4]). Querying paths with special constraints may shed light upon unknown before links between vertices, forming the basis for new hypotheses.

Possible application

Another example of graph structured data is metagenomic assemblies, and the problem is long subsequences detection and reconstruction. Some sequences have specific secondary structure, which can be described in terms of context-free grammar, and this grammar can be used for searching and classification. A lot of research in this area and tools are based on this approach, but most of them are only aimed at linear data processing. Despite the existence of tools for metagenomic assemblies analysis, context-free search in graph-structured assembly is still a challenge.

Possible application

Ontology	#triples	#results	GLL(ms)	sGPU(ms)
skos	252	810	10	12
generations	273	2164	19	13
travel	277	2499	24	30
univ-bench	293	2540	25	15
atom-primitive	425	15454	255	22
biomedical	459	15156	261	20
foaf	631	4118	39	9
people-pets	640	9472	89	32
funding	1086	17634	212	36
wine	1839	66572	819	54
pizza	1980	56195	697	24
g_1	8688	141072	1926	82
g_2	14712	532576	6246	185
g_3	15840	449560	7014	127

Acknowledgments

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References

- [1] Semyon Grigorev and Anastasiya Ragozina. Context-free path querying with structural representation of result. *arXiv preprint arXiv:1612.08872*, 2016.
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- [3] Petteri Sevon and Lauri Eronen. Subgraph queries by context-free grammars. *Journal of Integrative Bioinformatics (JIB)*, 5(2):157–172, 2008.
- [4] UniProt Consortium et al. Uniprot: a hub for protein information. *Nucleic acids research*, page gku989, 2014.