MODIFICATION OF VALIANT'S PARSING ALGORITHM FOR SUBSEQUENCES HANDLING

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Abstract. Some string-matching problems can be reduced to parsing: verification whether some subsequence can be derived in the given grammar. To apply parser-based solutions to such area as bioinformatics, one needs to improve parsing techniques ao that the processing of large amount of data were possible. The most asymptotically efficient parsing algorithm that can be applied to any context-free grammar is a matrix-based algorithm proposed by Valiant. This paper presents a modification of the Valiant's algorithm, which allows one to simplify highly parallel implementation, and efficiently utilize modern massively-parallel hardware. Moreover, the modified version decreases a large amount of excessive computations and accelerates the substrings searching.

1   Introduction

Secondary structure of genomic sequences prediction plays important role in classification and recognition problems. It comes from the idea that secondary structure is a source of information related with biological functions of various organisms.

Some approaches connected with secondary structure analysis based on using formal grammars, as they are successful in modeling strings with correlated symbols [1, 2]. That means the specific features of secondary structure can be described by some context-free grammar (CFG) and the prediction problem can be reduced to parsing—verification if some sequence can be derived in specified grammar. But checking the derivability is not frequently the main problem, sometimes all the derivable subsequences must be found [3].

The main disadvantage of CFG-based approaches is considerable problems with computational complexity. Traditional parsing method which is used in these approaches is CYK [4, 5] with cubic-time complexity, and this algorithm demonstrates poor performance on long strings or big grammars [6]. And so, as such field of application as bioinformatics requires working with a large amount of data, it is necessary to find more efficient parsing algorithms.

Still asymptotically most efficient parsing algorithm is based on matrix multiplication Valiant's algorithm [7]. Moreover, Okhotin generalized this algorithm to conjunctive and Boolean grammars which are the natural extensions of CFG with more expressive power [8]. For example, it is possible to express pseudoknots by using conjunctive grammars [9], while it is impossible by using context-free one. Valiant's algorithm allows to simply utilize parallel techniques to improve performance by offloading critical computations onto matrices multiplication. However, this algorithm is not appropriate for substrings finding problem.

In this paper we present the modification of Valiant's algorithm, which increases the power of using GPGPU and parallel computations by computing some matrices products concurrently. Also proposed algorithm can be easily adopted for the string-matching, or substring search, problem.

2 Formal langues

In this section we introduce basic definitions from formal language theory, and describe Valiant's parsing algorithm which we use as a base for our solution.

An alphabet Σ is a finite nonempty set of symbols. Σ^* is a set of all finite strings over Σ. A contex-free grammar G_S is a quadruple (Σ, N, R, S), where Σ is a finite set of terminals, N is a finite set of nonterminals, $\Sigma \cup N = \varnothing$, R is a finite set of productions of the form $A \to \beta$, where $A \in N, \beta \in V^*$, $V = \Sigma \cup N$ and $S \in N$ is a start symbol. Context-free grammar $G_S = (\Sigma, N, R, S)$ is said to be in Chomsky normal form if all productions in R are of the form: $A \to BC$, $A \to a$, $S \to \varepsilon$, where $A, B, C \in N, a \in \Sigma, \varepsilon$ is an empty string. $L_G(S) = \{\omega | S \xrightarrow[G_S]{*} \omega\}$ is a language specified by the grammar $G_S = (\Sigma, N, R, S)$, where $A \xrightarrow[G_S]{*} \omega$ means that ω can be derived in a finite number of rules applications from the start symbol S.

2.1 Valiant's parsing algorithm

Tabular parsing algorithms construct a matrix T cells of which are filled with nonterminals from which the corresponding substring can be derived. These algorithms are usually work with the grammar in Chomsky normal form. Namely, $T_{i,j} = \{A | A \in N, a_{i+1} \dots a_j \in L_G(A)\}$ $\forall i < j$, where $G_S = (\Sigma, N, R, S)$.

The elements of T are filled successively beginning with $T_{i-1,i} = \{A | A \to a_i \in R\}$. Then, $T_{i,j} = f(P_{i,j})$, where $P_{i,j} = \bigcup\limits_{k=i+1}^{j-1} T_{i,k} \times T_{k,j}$ and $f(P) = \{A | \exists A \to BC \in R : (B, C) \in P\}$. Finally, the input string $a_1 a_2 \dots a_n$ belongs to $L_G(S)$ iff $S \in T_{0,n}$.

If all elements are filled sequentially, the time complexity of this algorithm is $O(n^3)$. Valiant proposed to offload the most intensive computations to the Boolean matrix multiplication. As the most time-consuming is computing $\bigcup\limits_{k=i+1}^{j-1} T_{i,k} \times T_{k,j}$, Valiant anged the computation of $T_{i,j}$, in order to use multiplication of submatrices of T. Multiplication of two submatrices of parsing table T is defined as follows. Let $X \in (2^N)^{m \times l}$ and $Y \in (2^N)^{l \times n}$ be two submatrices of parsing table T. Then, $X \times Y = Z$, where $Z \in (2^{N \times N})^{m \times n}$ and $Z_{i,j} = \bigcup\limits_{k=1}^{l} X_{i,k} \times Y_{k,j}$.

Note that the computation of $X \times Y$ can be replaced by the multiplication of $|N|^2$ Boolean matrices (for each nonterminal pair). Denote the matrix corresponding to the pair $(B, C) \in N \times N$ as $Z^{(B,C)}$, then $Z_{i,j}^{(B,C)} = 1$ iff $(B, C) \in Z_{i,j}$. It should also be noted that $Z^{(B,C)} = X^B \times Y^C$. Each Boolean matrix multiplication can be computed independently. Following these changes, time complexity of this algorithm is $O(|G|BMM(n)log(n))$ for an input string of length n, where $BMM(n)$ is the number of operations needed to multiply two Boolean matrices of size $n \times n$.

Valiant's algorithm written as proposed by Okhotin is presented in listing 1. All elements of T and P are initialized by empty sets. Then, the elements of these two table are successively filled by two recursive procedures.

The procedure $compute(l, m)$ computes correct values of $T_{i,j}$ for all $l \le i < j < m$.

The procedure $complete(l, m, l', m')$ constructs the submatrix $T_{i,j}$ for all $l \le i < m$, $l' \le j < m'$. This procedure assumes $T_{i,j}$ for all $l \le i < j < m, l' \le i < j < m'$ are already constructed and the current value of $P[i,j] = \{(B,C) | \exists k, (m \le k < l'), a_{i+1} \dots a_k \in L(B), a_{k+1} \dots a_j \in L(C)\}$ for all $l \le i < m, l' \le j < m'$. The

Listing 1: Parsing by matrix multiplication: Valiant's Version

Input: Grammar $G = (\Sigma, N, R, S), w = a_1 \ldots a_n, n \geq 1, a_i \in \Sigma$, where $n + 1 = 2^k$

1 main():
2 *compute(0, n + 1);*
3 accept if and only if $S \in T_{0,n}$

4 compute(*l, m*):
5 **if** $m - l \geq 4$ **then**
6   *compute(l, $\frac{l+m}{2}$);*
7   *compute($\frac{l+m}{2}$, m)*
8 *complete(l, $\frac{l+m}{2}$, $\frac{l+m}{2}$, m)*

9 complete(*l, m, l′, m′*):
10 **if** $m - l = 4$ *and* $m = l'$ **then** $T_{l,l+1} = \{A|A \to a_{l+1} \in R\};$
11 **else if** $m - l = 1$ *and* $m < l'$ **then** $T_{l,l'} = f(P_{l,l'});$
12 **else if** $m - l > 1$ **then**
13      $leftgrounded = (l, \frac{l+m}{2}, \frac{l+m}{2}, m), rightgrounded = (l', \frac{l'+m'}{2}, \frac{l'+m'}{2}, m'),$
14      $bottom = (\frac{l+m}{2}, m, l', \frac{l'+m'}{2}), left = (l, \frac{l+m}{2}, l', \frac{l'+m'}{2}),$
15      $right = (\frac{l+m}{2}, m, \frac{l'+m'}{2}, m'), top = (l, \frac{l+m}{2}, \frac{l'+m'}{2}, m');$
16   complete(bottom);
17      $P_{left} = P_{left} \cup (T_{leftgrounded} \times T_{bottom});$
18   complete(left);
19      $P_{right} = P_{right} \cup (T_{bottom} \times T_{rightgrounded});$
20   complete(right);
21      $P_{top} = P_{top} \cup (T_{leftgrounded} \times T_{right});$
22      $P_{top} = P_{top} \cup (T_{left} \times T_{rightgrounded});$
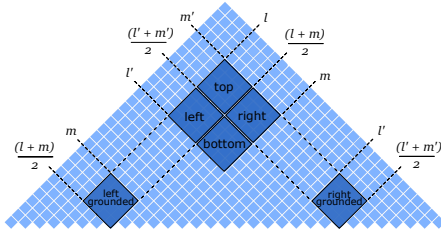23   complete(top)

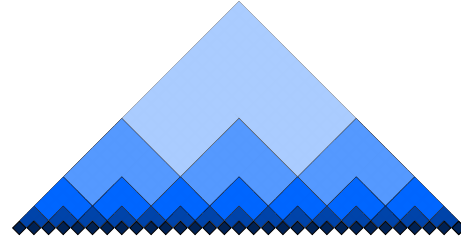Figure 1: Matrix partition used in *complete(l, m, l', m')* procedure.

Figure 2: Matrix partition on V-shaped layers used in modification.

submatrix division during the procedure call is shown in figure 2.

A simple example of parsing with the Valiant's algorithm is presented in figure 3. Only several steps is shown, but it is enough to point out at this version and our approach differences.

3 Modified Valiant's algorithm

In this section, we propose how to rearrange the order in which submatricess are precessed in the algorithm. The different order impreves independdence of submatrices handling and facilitates the implementation of parallel submatrix processing.

3.1 *Layered submatrices processing*

We propose to divide the parsing table into layers of disjoint submatrices of the same size (see figure 2). Such division is possible because derivation of substring of fixed length is not depended on left an right contexts. Appropriate order of substrings processing allows us to guarantyy disjointness of submatrices which form layer. Each layer
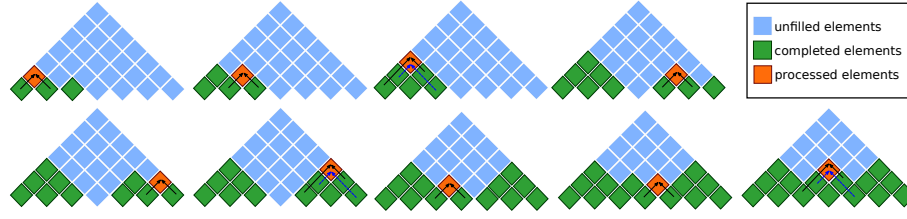
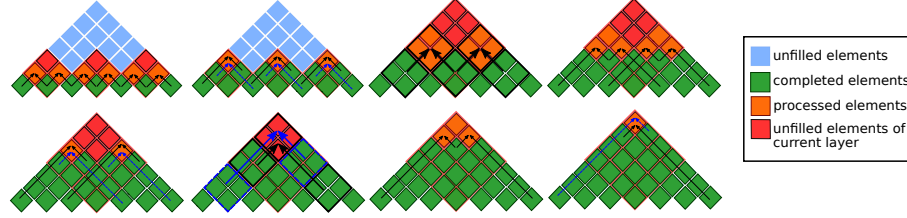Figure 3: An example of beginning of Valiant's algorithm

Figure 4: An example of the modification of Valiant's algorithm

consists of square matrices which size is a power of 2. The layers are computed successively in the bottom-up order. Each matrix in the layer can be handled independently, which facilitates parallelization of layer processing.

Figure 4 demonstartes the modified algorithm. The lowest layer (submatrices of size 1) has already been computed. The second layer is filled in in steps 1-2. Although the original algorithm computes the same matrix, the modified one needs two steps using parallel computation of submatrix products.

The modified version of Valiant's algorithm is presented in listing 2. The procedure *main()* computes the lowest layer $(T_{l,l+1})$, and then divides the table into layers, and computes them with the *completeVLayer()* function. Thus, *main()* computes all elements of parsing table T.

We define *left(subm)*, *right(subm)*, *top(subm)*, *bottom(subm)*, *rightgrounded(subm)* and *leftgrounded(subm)* functions which returns the submatrices for matrix $subm = (l, m, l', m')$ according to the original Valiant's algorithm (figure 2).

The procedure *completeVLayer(M)* takes an array of disjoint submatrices M which represents a layer. For each *subm = (l, m, l', m')* $\in M$ this procedure computes *left(subm), right(subm), top(subm)*. The procedure assumes that the elements of *bottom(subm)* and $T_{i,j}$ for all i and j such that $l \leq i < j < m$ and $l' \leq i < j < m'$ are already constructed. Also it is assumed that the current value of $P_{i,j} = \{(B,C) | \exists k, (m \leq k < l'), a_{i+1} \ldots a_k \in L_G(B), a_{k+1} \ldots a_j \in L_G(C)\}$ for all i and j such that $l \leq i < m$ and $l' \leq j < m'$.

The procedure *completeLayer(M)* also takes an array of disjoint submatrices M, but unlike the previous one, it computes $T_{i,j}$ for all $(i,j) \in subm$. This procedure requires exactly the same assumptions on $T_{i,j}$ and $P_{i,j}$ as in the previous case.

In other words, *completeVLayer(M)* computes the entire layer *M* and *completeLayer(M_2)* is a support function which is necessary for computation of smaller square submatrices $subm_2 \in M_2$ inside of *M*.

Finally, the procedure *performMultiplication(tasks)*, where *tasks* is an array of triples of submatrices, performs the basic step of algorithm: matrix multiplication. It is worth mentioning that $|tasks| \geq 1$ and each task can be computed independently, while the original algorithm handles one *task* per step sequentially. So, the practical implementation of this procedure can easily utilizes different techniques of parallel array processing, such as OpenMP.

3.2 *Algorithm for substrings*
Next, we show how our modification can be applied to the string-matching problem.

Listing 2: Parsing by matrix multiplication: Modified Version

Input: $G = (\Sigma, N, R, S), w = a_1 \ldots a_n, n \geq 1, n + 1 = 2^p, a_i \in \Sigma$

1 main():
2 **for** $l \in \{1, \ldots, n\}$ **do** $T_{l,l+1} = \{A | A \to a_{l+1} \in R\}$;
3 **for** $1 \leq i < p - 1$ **do**
4   layer = *constructLayer(i)*;
5   *completeVLayer(layer)*
6 accept if and only if $S \in T_{0,n}$

7 constructLayer(i):

8 $\{(k2^i, (k+1)2^i, (k+1)2^i, (k+2)2^i) \,|\, 0 \leq k < 2^{p-i} - 1\}$

9 completeLayer(M):

10 **if** $\forall (l, m, l', m') \in M \quad (m - l = 1)$ **then**
11   **for** $(l, m, l', m') \in M$ **do** $T_{l,l'} = f(P_{l,l'})$;
12 **else**
13   *completeLayer($\{bottom(subm) \,|\, subm \in M\}$)*;
14   *completeVLayer(M)*

15 completeVLayer(M):

16 *multiplicationTasks$_1$ =*
     $\{left(subm), leftgrounded(subm), bottom(subm) \,|\, subm \in M\} \cup$
     $\{right(subm), bottom(subm), rightgrounded(subm) \,|\, subm \in M\}$;

17 multiplicationTask$_2$ = $\{top(subm), leftgrounded(subm), right(subm) \,|\, subm \in M\}$;

18 multiplicationTask$_3$ = $\{top(subm), left(subm), rightgrounded \,|\, subm \in M\}$;

19 *performMultiplications(multiplicationTask$_1$)*;
20 *completeLayer($\{left(subm) \,|\, subm \in M\} \cup \{right(subm) \,|\, subm \in M\}$)*;
21 *performMultiplications(multiplicationTask$_2$)*;
22 *performMultiplications(multiplicationTask$_3$)*;
23 *completeLayer($\{top(subm) \,|\, subm \in M\}$)*

24 performMultiplication(tasks):
25 **for** $(m, m1, m2) \in tasks$ **do** $P_m = P_m \cup (T_{m1} \times T_{m2})$;

To find all substrings of size s, which can be derived from a start symbol for an input string of size $n = 2^p$, we need to compute layers with submatrices of size not greater than $2^{l'}$, where $2^{l'-2} < s \leq 2^{l'-1}$.

Let $l' = p - (m - 2)$ and consequently $(m - 2) = p - l'$. For any $m \leq i \leq p$ products of submatrices of size 2^{p-i} are calculated exactly $2^{2i-1} - 2^i$ times and each of them imply multiplying $\mathcal{O}(|G|)$ Boolean submatrices.

$$C \sum_{i=m}^{p} 2^{2i-1} \cdot 2^{\omega(p-i)} \cdot f(2^{p-i}) = C \cdot 2^{\omega l'} \sum_{i=2}^{l'} 2^{(2-\omega)i} \cdot 2^{2(p-l')-1} \cdot f(2^{l'-i}) \leq$$

$$C \cdot 2^{\omega l'} f(2^{l'}) \cdot 2^{2(p-l')-1} \sum_{i=2}^{l'} 2^{(2-\omega)i} = BMM(2^{l'}) \cdot 2^{2(p-l')-1} \sum_{i=2}^{l'} 2^{(2-\omega)i}$$

Thus, time complexity for searching all substrings is $O(|G|BMM(2^{l'})(l'-1))$, while time complexity for the full input string is $O(|G|BMM(2^p)(p-1))$. In contract to the modification, Valiant's algorithm completely calculate at least 2 triangle submatrices of size $\frac{n}{2}$ (as shown in figure 5) which means the minimum asymptotic complexity is $O(|G|BMM(2^{p-1})(p-2))$. Thus we can conclude that the modification is asymptotically faster for substrings of size $s \ll n$ than the original algorithm.
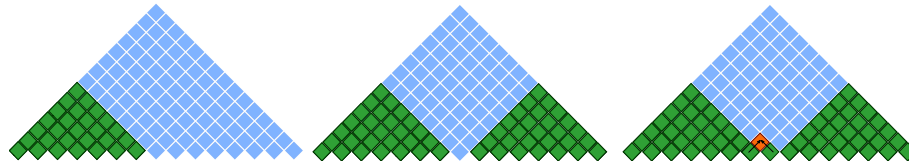
Figure 5: The number of elements necessary to compute in Valiant's algorithm. That means it is nessesary to calculate at least 2 triangle submatrices of size $\frac{n}{2}$.

4   Conclusion

We presented the modification of Valiant's algorithm, which makes it possible to use parallel computations more effectively. Also we showed its applicability to the string-matching problem the original algorithm was not able to deal with.

The directions for future research are high-performance implementation using GPGPU or other parallel techniques and its evaluation on the real-world data.

Also we plan to extend the proposed algorithm for conjunctive and boolean grammars handling. It should be useful for complex secondary structure features processing.

Acknowledgments

References

[1] B. Knudsen and J. Hein, "Rna secondary structure prediction using stochastic context-free grammars and evolutionary history.," *Bioinformatics (Oxford, England)*, vol. 15, no. 6, pp. 446–454, 1999.

[2] R. D. Dowell and S. R. Eddy, "Evaluation of several lightweight stochastic context-free grammars for rna secondary structure prediction," *BMC bioinformatics*, vol. 5, no. 1, p. 71, 2004.

[3] R. Durbin, S. Eddy, A. Krogh, and G. Mitchison, *Biological sequence analysis*. Cambridge University Press, 1996.

[4] T. Kasami, "An efficient recognition and syntax-analysis algorithm for context-free languages," *Coordinated Science Laboratory Report no. R-257*, 1966.

[5] D. H. Younger, "Context-free language processing in time n3," in *Proceedings of the 7th Annual Symposium on Switching and Automata Theory (Swat 1966)*, SWAT '66, (Washington, DC, USA), pp. 7–20, IEEE Computer Society, 1966.

[6] T. Liu and B. Schmidt, "Parallel rna secondary structure prediction using stochastic context-free grammars," *Concurrency and Computation: Practice and Experience*, vol. 17, no. 14, pp. 1669–1685, 2005.

[7] L. G. Valiant, "General context-free recognition in less than cubic time," *J. Comput. Syst. Sci.*, vol. 10, pp. 308–315, Apr. 1975.

[8] A. Okhotin, "Parsing by matrix multiplication generalized to boolean grammars," *Theor. Comput. Sci.*, vol. 516, pp. 101–120, Jan. 2014.

[9] R. Zier-Vogel and M. Domaratzki, "Rna pseudoknot prediction through stochastic conjunctive grammars," *Computability in Europe 2013. Informal Proceedings*, pp. 80–89, 2013.