

# AUTHOR'S GUIDELINES FOR CIBB PAPERS

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**Abstract.** The theory of formal languages and, particularly, context-free grammars has been extensively studied and applied in different areas. For example, several approaches to the recognition and classification problems in bioinformatics are based on searching the genomic subsequences possessing some specific features which can be described by a context-free grammar. Therefore, the string-matching problem can be reduced to parsing verification if some subsequence can be derived in this grammar. Such field of application as bioinformatics requires working with a large amount of data, so it is necessary to improve the existing parsing techniques. 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 aims to present Valiants algorithm modification, which main advantage is the possibility to divide the parsing table into successively computed layers of disjoint submatrices where each submatrix of the layer can be processed independently. Moreover, our approach is easily adapted for the string-matching problem. Our evaluation shows that the proposed modification retains all benefits of Valiants algorithm, especially its high performance achieved by using fast matrix multiplication methods. Also, the modified version decreases a large amount of excessive computations and accelerates the substrings searching.

## 1 Introduction

Recent research has shown that the theory of formal languages and, in particular, context-free languages can be used in bioinformatics [?, ?, ?, ?]. ....

A good example of this usage is the recognition and classification problems in bioinformatics, some of them are based on the research claiming that the secondary structure of the DNA and RNA nucleotide sequence contains important information about the organism species. The specific features of the secondary structure can be described by some context-free grammar, and therefore the recognition problem can be reduced to parsing—verification if some nucleotide sequence can be derived in this grammar.

Such field of application as bioinformatics requires working with a large amount of data, so it is necessary to find highly efficient parsing algorithm.

The majority of parsing algorithms either has the cubic-time complexity (Kasami [?], Younger [?], Earley [?]) or could work only with sub-classes of context-free grammars (Bernardy, Claussen [?]), but still asymptotically more efficient parsing algorithm that can be applied to any context-free grammar is algorithm based on matrix multiplication proposed by Leslie Valiant [?]. Moreover, Okhotin generalized this algorithm to conjunctive and Boolean grammars which are the natural extensions of context-free grammars with more expressive power [?].

In this paper, we propose the modification of Valiant's algorithm which allows to compute some matrix products concurrently and show the applicability of our approach in bioinformatics research, especially in addressing the string-matching problem.

## 2 Scientific Background

### 2.1 Preliminaries

An alphabet  $\Sigma$  is a finite nonempty set of symbols.  $\Sigma^*$  is a set of all finite strings over  $\Sigma$ . A grammar is a quadruple  $(\Sigma, N, R, S)$ , where  $\Sigma$  is a finite set of terminals,  $N$  is a finite set of nonterminals,  $R$  is a finite set of productions of the form  $\alpha \rightarrow \gamma$ , where  $\alpha \in V^*NV^*$ ,  $\gamma \in V^*$ ,  $V = \Sigma \cup N$  and  $S \in N$  is a start symbol.

Grammar  $G = (\Sigma, N, R, S)$  is called context-free, if  $\forall r \in R$  are of the form  $A \rightarrow \beta$ , where  $A \in N, \beta \in V^*$ .

Context-free grammar  $G = (\Sigma, N, R, S)$  is said to be in Chomsky normal form if all productions in  $R$  are of the form:

- $A \rightarrow BC$ ,
- $A \rightarrow a$ ,
- $S \rightarrow \varepsilon$ , where  $A, B, C \in N, a \in \Sigma, \varepsilon$  is an empty string.

$L_G(A)$  is a language of the grammar  $G_A = (\Sigma, N, R, A)$ , which means all the sentences that can be derived in a finite number of rules applications from the start symbol  $A$ .

### 2.2 Parsing by matrix multiplication

The main problem of parsing is to verify if the input string belongs to the language of some given grammar  $G$ .

This work is based on parsing algorithm presented by Valiant[]. Main idea of all tabular parsing methods is to construct a parsing table  $T$  of size  $(n + 1) \times (n + 1)$  for an input string  $a_1a_2 \dots a_n$  and context-free grammar  $G = (\Sigma, N, R, S)$  which is in Chomsky normal form, where

$$T_{i,j} = \{A | A \in N, a_{i+1} \dots a_j \in L_G(A)\} \quad \forall i < j. \quad (1)$$

The elements of  $T$  are filled successively beginning with

$$T_{i-1,i} = \{A | A \rightarrow a_i \in R\} \quad (2)$$

Then,

$$T_{i,j} = f(P_{i,j}), \quad (3)$$

where

$$P_{i,j} = \bigcup_{k=i+1}^{j-1} T_{i,k} \times T_{k,j} \quad (4)$$

$$f(P) = \{A | \exists A \rightarrow BC \in R : (B, C) \in P\} \quad (5)$$

The input string  $a_1a_2 \dots a_n$  belongs to  $L_G(S)$  if and only if  $S \in T_{0,n}$ .

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  $\bigcup_{k=i+1}^{j-1} T_{i,k} \times T_{k,j}$ , Valiant rearranged computation of  $T_{i,j}$ , in order to use multiplication of submatrices of  $T$ .

Firstly, define multiplication of two submatrices of parsing table  $T$ . 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  $Z_{i,j} = \bigcup_{k=1}^l X_{i,k} \times Y_{k,j}$ .

And next,  $X \times Y = Z$  can be replaced by multiplication of  $|N|^2$  Boolean matrices (for each nonterminal pair). Denote matrix corresponding to pair  $(B, C) \in N \times N$  as  $Z^{(B,C)}$ , then  $Z_{i,j}^{(B,C)} = 1$  if and only if  $(B, C) \in Z_{i,j}$ . 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  $n \times n$ .

In listing 1 full pseudo-code of Valiant's algorithm is written in the terms proposed by Okhotin, is presented. 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.

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

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**Input:** Grammar  $G = (\Sigma, N, R, S)$ ,  $w = a_1 \dots a_n$ ,  $n \geq 1$ ,  $a_i \in \Sigma$ , where  $n + 1$  is a power of two

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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
11    $T_{l,l+1} = \{A | A \rightarrow a_{l+1} \in R\}$ ;
12 else if  $m - l = 1$  and  $m < l'$  then
13    $T_{l,l'} = f(P_{l,l'})$ ;
14 else if  $m - l > 1$  then
15   leftgrounded = ( $l, \frac{l+m}{2}, \frac{l+m}{2}, m$ ), rightgrounded = ( $l', \frac{l'+m'}{2}, \frac{l'+m'}{2}, m'$ ),
16   bottom = ( $\frac{l+m}{2}, m, l', \frac{l'+m'}{2}$ ), left = ( $l, \frac{l+m}{2}, l', \frac{l'+m'}{2}$ ),
17   right = ( $\frac{l+m}{2}, m, \frac{l'+m'}{2}, m'$ ), top = ( $l, \frac{l+m}{2}, \frac{l'+m'}{2}, m'$ );
18   complete(bottom);
19    $P_{left} = P_{left} \cup (T_{leftgrounded} \times T_{bottom})$ ;
20   complete(left);
21    $P_{right} = P_{right} \cup (T_{bottom} \times T_{rightgrounded})$ ;
22   complete(right);
23    $P_{top} = P_{top} \cup (T_{leftgrounded} \times T_{right})$ ;
24    $P_{top} = P_{top} \cup (T_{left} \times T_{rightgrounded})$ ;
25   complete(top)
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The procedure  $compute(l, m)$  constructs the correct values of  $T_{i,j}$  for all  $l \leq i < j < m$ .

The procedure  $complete(l, m, l', m')$  constructs the submatrix  $T_{i,j}$  for all  $l \leq i < m$ ,  $l' \leq j < m'$ . This procedure assumes  $T_{i,j}$  for all  $l \leq i < j < m$ ,  $l' \leq i < j < m'$  are already constructed and the current value of  $P[i, j] = \{(B, C) | \exists k, (m \leq k < l'), a_{i+1} \dots a_k \in L(B), a_{k+1} \dots a_j \in L(C)\}$  for all  $l \leq i < m$ ,  $l' \leq j < m'$ . The submatrix division during the procedure call is shown in figure 2.

In figure 3 is presented a simple example of Valiant's algorithm. Only the beginning of the work is shown, because later we point out at this version and our approach differences.

### 3 Modified Valiant's algorithm

In this section we describe the reorganization of submatrix processing order in the Valiant's algorithm which simplify independent handling of submatrices. As a result, proposed modification can facilitate implementation of parallel submatrix processing.

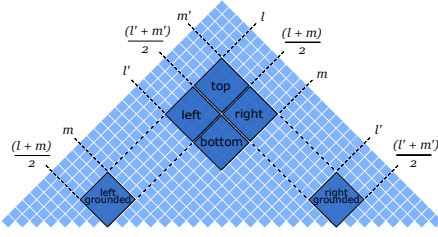


Figure 1: Matrix partition used in *complete*( $l, m, l', m'$ ) procedure.

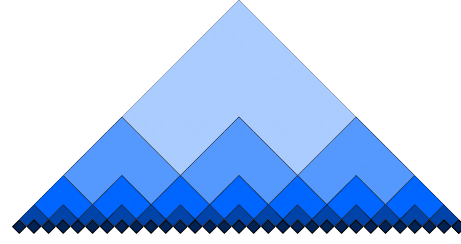


Figure 2: Matrix partition on V-shaped layers used in modification.

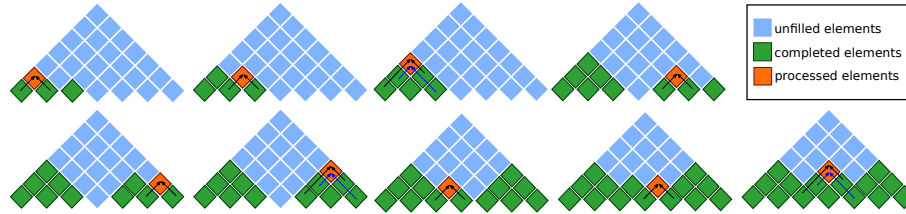


Figure 3: An example of beginning of Valiant's algorithm

### 3.1 New approach

The main change of this modification is the possibility to divide the parsing table into layers of disjoint submatrices of the same size. The idea of division we have made from the reorganization of the matrix multiplication order is presented in figure 2. Each layer consists of square matrices which size is power of 2. The layers are computed successively in the bottom-up order. Each matrix in the layer can be handled independently, which can help to implement parallel version of layer processing function.

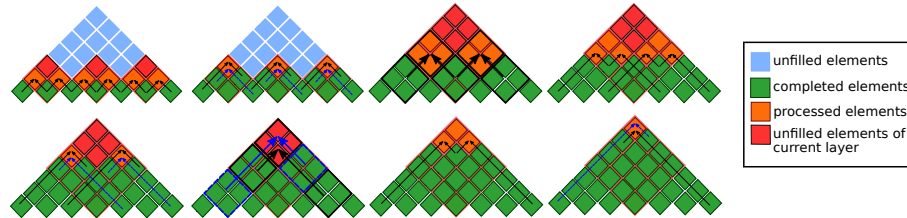


Figure 4: An example of the modification of Valiant's algorithm

A simple example of the modification is shown in figure 4. The lowest layer (submatrices which size is 1) is already computed and filling of the matrix starts with the second layer (subfigures 1-2). Note that the same process is presented in figure 3, but here it can be done only in 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 divide the table into layers, described earlier, and computes them through the *completeVLayer*() call. Thus, *main*() computes all elements of parsing table  $T$ . (Hereinafter, we use layer to mean set of submatrices.)

For brevity, 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).

Also denote some subsidiary functions for matrix layer  $M$ :

- $bottomsublayer(M) = \{bottom(subm) \mid subm \in M\}$ ,
- $leftsublayer(M) = \{left(subm) \mid subm \in M\}$ ,
- $rightsublayer(M) = \{right(subm) \mid subm \in M\}$ ,
- $topsublayer(M) = \{top(subm) \mid subm \in M\}$ .

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

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**Listing 2: Parsing by matrix multiplication: Modified Version**

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

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```

1 main():
2 for  $l \in \{1, \dots, n\}$  do
3    $T_{l,l+1} = \{A \mid A \rightarrow a_{l+1} \in R\}$ 
4 for  $1 \leq i < p - 1$  do
5    $\text{layer} = \text{constructLayer}(i);$ 
6    $\text{completeVLayer}(\text{layer})$ 
7 accept if and only if  $S \in T_{0,n}$ 
8 constructLayer(i):
9  $\{(k2^i, (k+1)2^i, (k+1)2^i, (k+2)2^i) \mid 0 \leq k < 2^{p-i} - 1\}$ 
10 completeLayer(M):
11 if  $\forall (l, m, l', m') \in M \quad (m - l = 1)$  then
12   for  $(l, m, l', m') \in M$  do
13      $T_{l,l'} = f(P_{l,l'});$ 
14 else
15    $\text{completeLayer}(\text{bottomsublayer}(M));$ 
16    $\text{completeVLayer}(M)$ 
17 completeVLayer(M):
18  $\text{multiplicationTasks}_1 =$ 
    $\{left(subm), leftgrounded(subm), bottom(subm) \mid subm \in M\} \cup$ 
    $\{right(subm), bottom(subm), rightgrounded(subm) \mid subm \in M\};$ 
19  $\text{multiplicationTask}_2 = \{top(subm), leftgrounded(subm), right(subm) \mid subm \in M\};$ 
20  $\text{multiplicationTask}_3 = \{top(subm), left(subm), rightgrounded \mid subm \in M\};$ 
21  $\text{performMultiplications}(\text{multiplicationTask}_1);$ 
22  $\text{completeLayer}(leftsublayer(M) \cup rightsublayer(M));$ 
23  $\text{performMultiplications}(\text{multiplicationTask}_2);$ 
24  $\text{performMultiplications}(\text{multiplicationTask}_3);$ 
25  $\text{completeLayer}(topsublayer(M))$ 
26 performMultiplication(tasks):
27 for  $(m, m1, m2) \in \text{tasks}$  do
28    $P_m = P_m \cup (T_{m1} \times T_{m2});$ 
```

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$left(subm)$ ,  $right(subm)$ ,  $top(subm)$ . 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  $P_{i,j} = \{(B, C) \mid \exists k, (m \leq k < l'), a_{i+1} \dots a_k \in L_G(B), a_{k+1} \dots a_j \in L_G(C)\}$  for all  $i$  and  $j$  such that  $l \leq i < m$  and  $l' \leq j < m'$ .

The procedure  $\text{completeLayer}(M)$  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 same assumptions on  $T_{i,j}$  and  $P_{i,j}$  as in the previous case.

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

Finally, the procedure  $\text{performMultiplication}(tasks)$ , where  $tasks$  is an array of a triple of submatrices, perform basic step of algorithm: matrix multiplication. It is worth mentioning that, as distinct from the original algorithm, here  $|tasks| \geq 1$  and each task can be computed independently. So, practical implementation of this procedure can easily involve 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.

So if we want 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.

$$\begin{aligned}
C \sum_{i=m}^p 2^{2i-1} \cdot 2^{\omega(p-i)} \cdot f(2^{p-i}) &= C \cdot 2^{\omega l'} \sum_{i=2}^{l'} 2^{(2-\omega)i} \cdot 2^{2(p-l')-1} \cdot f(2^{l'-i}) \leq \\
C \cdot 2^{\omega l'} f(2^{l'}) \cdot 2^{2(p-l')-1} \sum_{i=2}^{l'} 2^{(2-\omega)i} &= BMM(2^{l'}) \cdot 2^{2(p-l')-1} \sum_{i=2}^{l'} 2^{(2-\omega)i}
\end{aligned} \tag{6}$$

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 contrast to the modification, Valiant's algorithm completely calculate at least 2 triangle submatrices of size  $\frac{n}{2}$  (as shown in figure 5) which mean minimum asymptotic complexity  $O(|G|BMM(2^{p-1})(p - 2))$ . Make a conclusion that the modification is asymptotically faster for substrings of size  $s \ll n$  than the original algorithm.

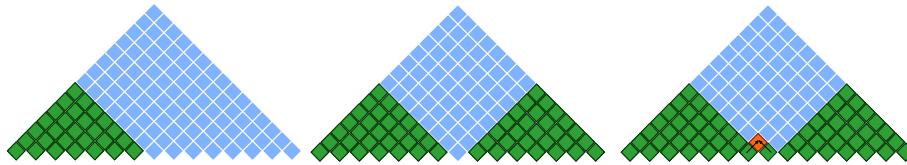


Figure 5: The number of elements necessary to compute in Valiant’s algorithm. That means it is necessary to calculate at least 2 triangle submatrices of size  $\frac{n}{2}$ .

### 3.3 Evaluation

After demonstrating the theoretical value of the proposed solution, the next step of our work was to show its applicability on real data. Both algorithms (original Valiant’s version and the modification) were compared on context-free grammar  $G$  ...?picture?... which is used to approximate the secondary structure of the biological sequences. As it was mentioned before, the secondary structure is a very powerful instrument for species classification and identification problem. Parsing algorithms based on matrix multiplication helps efficiently find subsequences with features specific to the secondary structure.

The algorithms were implemented using a library for fast Boolean matrix multiplication M4RI [?]. The biological sequences were taken from this dataset[.]

All tests were run on a PC with the following characteristics:

- OS:
- CPU:
- System Type:
- RAM:

The results of experiments which are presented "...? show that our modification can be efficiently applied to the string matching problem as it demonstrates good time on real data.

## 4 Conclusion

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### **Acknowledgments**

Example of the Acknowledgments section.

### **References**