Finding Maximal Exact Matches in Graph

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Contents

Prerequisites
BWT Transform: Pseudocode

Assuming our strings' indices are 1-based, we now give a non-efficient algorithm to calculate the BWT transform of a string.

```
def BWT(s: str) -> str:
        T = []
        for character in s:
                s = s[len(s)] + s[1..len(s)-1]
                T.push(s)
        sort_lexicographically(T)
        return last_column(T)
```

Prerequisites

BWT Transform: Example

Transformation				
1. Input	2. All rotations	3. Sort into lexical order	4. Take the last column	5. Output
BANANA$	BANANA$ $BANANA A$BANAN NA$BANA ANA$BAN NANA$BA ANANA$B BANANA$	$BANANA BANANA$ A$BANAN ANA$BAN ANANA$B BANANA$ NA$BANA NANA$BA	$BANANA BANANA$ A$BANAN ANA$BAN ANANA$B BANANA$ NA$BANA NANA$BA	A$NNBAA

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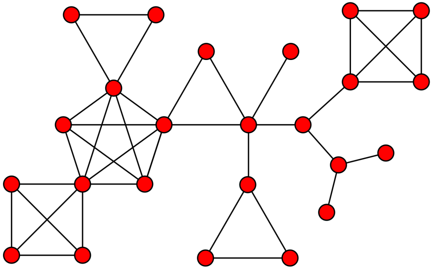
Definition (Block Graph)

We call **block graph** an undirected graph in which every biconnected component (i.e. a **block**) is a clique.



Definition (Elastic Founder Graph)

Consider a block graph $G = (V, E, l)$ with $l : V \rightarrow \Sigma^+$. We call such a graph an **indexable Elastic Founder Graph** if the **semi-repeat-free** property holds: for each v in block V_i, $l(v)$ occurs in G only as prefix of paths starting with some $w \in V_i$.

Let $Q \in \Sigma^+$ be a query string, κ be a threshold, $lext(i, P, j)$ the left extension of the string $P[i..j]$ and $rext(i, P, j)$ the right extension.

Definition (LEFTMAX)

A match $([x..y], (i, P, j))$ of $Q[x..y]$ in G satisfies the *LEFTMAX* property if and only if

$$x = 1 \ \vee \ lext(i, P, j) = \emptyset \ \vee \ Q[x-1] \notin lext(i, P, j)$$

We can analogously define the RIGHTMAX property.

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We can analogously define the RIGHTMAX property.

Definition (κ-MEM)

A match $([x..y], (i, P, j))$ of $Q[x..y]$ in G is called a κ-MEM if it satisfies all the following conditions:

1. $LEFTMAX \vee |lext(i, P, j)| \geq 2$
2. $RIGHTMAX \vee |rext(i, P, j)| \geq 2$
3. $y - x + 1 \geq \kappa$

MEMs in Node Labels

Node MEMs: definition

Definition (Node MEM)

A κ-MEM between a query string Q and the label $l(v)$ of a vertex $v \in V$ is called a node-MEM.

To give an algorithm to find node-MEMs we must consider the text

$$T_{\text{nodes}} = \prod_{v \in V} 0 \times l(v).$$

We also need a data structure supporting the following operations over a bitvector B:

1. `r = rank(B, i)` in $O(1)$ with $r = \sum_{j=1}^{i} B[j]$,
2. `j = select(B, r)` in $O(1)$ with $j \leq i$ the position of the r-th 1 in B.

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We assume we have at our disposal the following procedures:

1. `mems_using_bidirectional_bwts` which takes as input two bidirectional BWT indices on strings T, Q and a threshold κ and outputs Q' MEM strings with $|Q'| \geq \kappa$ and for each string Q' four BWT intervals $([i_T..j_T], [i'_T..j'_T], [i_Q..j_Q], [i'_Q..j'_Q])$ which represent the maximal matches of T and Q in $O(|T| + |Q|)$ time;
2. `mems_from_bidirectional_bwt` which takes as input four BWT intervals and outputs the corresponding MEM string Q' in $O(|Q'|)$.

For both of these algorithms, one may refer to Algorithm 11.3 and Algorithm 11.4 from Genome-Scale Algorithm Design: Biological Sequence Analysis in the Era of High-Throughput Sequencing (Belazzougui et alia).

MEMs in Node Labels

Algorithm to find k-node MEMs: prerequisites

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MEMs in Node Labels

Algorithm to find k-node MEMs

We can now describe the algorithm to find node MEMs.

1. We build a bitvector B to mark the location of 0s in T_{nodes} so that with the rank operation we can identify the corresponding node in G.
2. We call `mems_using_bidirectional_bwts` using bidirectional BWT indices on strings T_{nodes} and Q.
3. For each string Q' we get, we call `mems_from_bidirectional_bwt` on its corresponding BWT intervals.
4. We use B to obtain the tuple (i, P, j) in $O(1)$ time.

The algorithm described above has complexity $O(|T_{\text{nodes}}| + |Q| + N_{\kappa})$ with N_{κ} the number of output MEMs.

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k-Node MEMs spanning exactly L nodes

Algorithm to find k-Node MEMs spanning exactly L nodes: prerequisites

1. We call P_G^L a path of G spanning exactly L nodes.
2. We define two new symbols c and d not originally part of the alphabet Σ and the two operators:

$$left(u) = \begin{cases} c \text{ if } lext(u) = \{c\} \\ \# \text{ otherwise} \end{cases}$$

$$right(u) = \begin{cases} d \text{ if } rext(u) = \{d\} \\ \# \text{ otherwise} \end{cases}$$

3. We define the text

$$T_L = 0 \times \prod_{u_1,..,u_L \in P_G^L} \left(left(u_1) \times l(u_1) \times \cdots \times l(u_L) \times right(u_L) \times 0 \right).$$

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k-Node MEMs spanning exactly L nodes

Algorithm to find k-Node MEMs spanning exactly L nodes

1. We modify the `mems_from_bidirectional_bwt` so that it makes use of the symbols defined before we get the result using the algorithm we defined for κ-node MEMs.
2. The complexity we get is $O(|T_L| + |Q| + M_{\kappa,L})$ with $M_{\kappa,L}$ the number of output MEMs.
3. Let d be the maximum in-degree (or out-degree) of a node, n the total label length of G. Now we can reformulate the time complexity.
4. $|T_L|$ is the concatenation of paths of G of length L: for a node v the number of paths containing $l(v)$ is at most $L \times d^{L-1}$. The complexity can be rewritten as $O(|Q| + M_{\kappa,L} + n \times L \times d^{L-1})$ which is exponential on L.

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MEMs in EFGs

k-Node MEMs in EFGs: Remark

Remark

Given an indexable EFG $G = (V, E, l)$, for each $(v, w) \in E$ string $l(v)l(w)$ occurs only as prefix of paths starting with v.

Rephrasing what is written above, all occurrences of some string S in G spanning at least four nodes can be decomposed as $\alpha l(u_2) \dots l(u_{L-1})\beta$ such that:

1. $u_2 \dots u_{L-1}$ is a path in G and $u_2, \dots, u_{L-1}$ are unequivocally identified;
2. $\alpha = l(u_1)[i..||u_1||]$ with $1 \le i \le ||u_1||$ for some $(u_1, u_2) \in E$;
3. $\beta = l(u_L)$ for some $(u_{L-1}, u_L) \in E$ or $\beta = l(uL)(l(uL+1)[1..j])$ with $1 \le j \le ||u_{L+1}||$ for some $(u_{L-1}, u_L), (u_L, u_{L+1}) \in E$.

Note that $\alpha, \beta \neq \epsilon$ and β has as prefix a full node label, α might spell any suffix of a node label.

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Note that $\alpha, \beta \neq \epsilon$ and β has as prefix a full node label, α might spell any suffix of a node label.

First, we take the text $T_3' = \prod_{(u,v),(v,w)\in E}\big(l(u)l(v)l(w) \times 0\big)$.

1. We mark all implicit or explicit nodes $\bar{p}$ such that the corresponding root-to-$\bar{p}$ path spells $l(u)l(v)$ for some $(u, v) \in E$, so that we can query in constant time if $\bar{p}$ is such a node.
2. We compute pointers from each node $\bar{p}$ to an arbitrarily chosen leaf in the subtree rooted at $\bar{p}$;
3. for each node $v \in V$ of the indexable EFG we build trie T_v for the set of strings $\overline{l(u)} : (u, v) \in E$;
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MEMs in EFGs

k-Node MEMs in EFGs spanning more than 3 nodes: preprocessing

First, we take the text $T_3' = \prod_{(u,v),(v,w)\in E}\left(l(u)l(v)l(w) \times 0\right)$.

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Let $\bar{p}$ be the suffix tree node of T'_3 reached from the root by spelling $Q[1..y]$ in the suffix tree until we cannot continue with $Q[y+1]$:

1. If we cannot continue with a 0, $Q[1..y]$ spans no more than 3 nodes, so we can discard it. We can now consider matching $Q[2..y]$ in G taking the suffix link of $\bar{p}$.
2. If we can continue with a 0 and the occurrences of $Q[1..y]$ span no more than 2 nodes, we proceed as in the previous step.
3. In this case, $Q[1..y] = \alpha l(u_2)l(u_3)$ for exactly one $u_2 \in V$, with $(u_2, u_3) \in E$, we follow the suffix link walk from $\bar{p}$ until we find the marked node $\bar{q}$ corresponding to $l(u_2)l(u_3)$: from $\bar{q}$ we try to match $Q[y+1..]$ until failure, matching $Q[y+1..y']$ and reaching node $\bar{r}$.

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3. In this case, $Q[1..y] = \alpha l(u_2)l(u_3)$ for exactly one $u_2 \in V$, with $(u_2, u_3) \in E$, we follow the suffix link walk from $\bar{p}$ until we find the marked node $\bar{q}$ corresponding to $l(u_2)l(u_3)$: from $\bar{q}$ we try to match $Q[y+1..]$ until failure, matching $Q[y+1..y']$ and reaching node $\bar{r}$.

MEMs in EFGs

k-Node MEMs in EFGs spanning more than 3 nodes: processing

Let $\bar{p}$ be the suffix tree node of T'_3 reached from the root by spelling $Q[1..y]$ in the suffix tree until we cannot continue with $Q[y+1]$:

1. If we cannot continue with a 0, $Q[1..y]$ spans no more than 3 nodes, so we can discard it. We can now consider matching $Q[2..y]$ in G taking the suffix link of $\bar{p}$.
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Theorem (Algorithm complexity)

Let alphabet Σ be of constant size, and let $G = (V, E, l)$ be an indexable Elastic Founder Graph of height H, that is, the maximum number of nodes in a block of G is H. The algorithm to find κ-node-MEMs spanning $L > 3$ nodes has time complexity $O(nH^2 + |Q| + M_\kappa)$ with $n = \sum_{v \in V} |v|$ and M_κ the number of output MEMs.

Proof.

It derives from the complexity of the algorithm to find κ-node MEMs spanning exactly L nodes given before. □

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Corollaries

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The results we have given for κ-node MEMs, κ-node MEMs spanning exactly L nodes and EFGs hold when $Q[1..m]$ is replaced by a set of queries of total length m.

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The algorithms we have given before (including the corollary above) can be modified to report only MEMs that occur in text T formed by concatenating the rows (ignoring gaps and adding separator symbols) of the input MSA of the indexable EFG.

This can be done in additional $O(|T| + r \log r)$ time and $O(r \log n)$ bits of space, and with multiplicative factor $O(\log \log n)$ added to the running times of the respective algorithms, where r is the number of equal-letter runs in the BWT of T.

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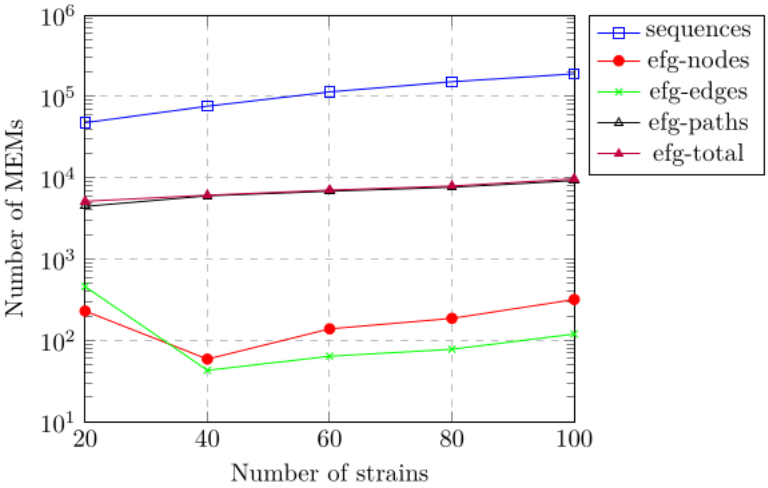
Experimental results

Number of MEMs with different indices and varying number of covid19 strains



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