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Minimum Segmentation for Pan-genomic Founder Reconstruction in Linear Time

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Abstract
Given a threshold \( L \) and a set \( \mathcal{R} = \{R_1, \ldots, R_m\} \) of \( m \) strings (haplotype sequences), each having length \( n \), the minimum segmentation problem for founder reconstruction is to partition \([1, n]\) into set \( P \) of disjoint segments such that each segment \([a, b] \in P\) has length at least \( L \) and the number \( d(a, b) = |\{R_i[a, b] : 1 \leq i \leq m\}| \) of distinct substrings at segment \([a, b]\) is minimized over \([a, b] \in P\). The distinct substrings in the segments represent founder blocks that can be concatenated to form \( \max\{d(a, b) : [a, b] \in P\} \) founder sequences representing the original \( \mathcal{R} \) such that crossovers happen only at segment boundaries. We give an optimal \( O(mn) \) time algorithm to solve the problem, improving over earlier \( O(mn^2) \). This improvement enables to exploit the algorithm on a pan-genomic setting of input strings being aligned haplotype sequences of complete human chromosomes, with a goal of finding a representative set of references that can be indexed for read alignment and variant calling. We implemented the new algorithm and give some experimental evidence on the practicality of the approach on this pan-genomic setting.

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1 Introduction

A key problem in pan-genomics is to develop a sufficiently small, efficiently queriable, but still descriptive representation of the variation common to the subject under study [1]. For example, when studying human population, one would like to take all publicly available
variation datasets (e.g. [19, 4, 20]) into account. Many approaches encode the variation as a graph [16, 9, 18, 2, 10, 8] and then one can encode the different haplotypes as paths in this graph [13, 17]. An alternative was proposed in [22], based on a compressed indexing scheme for a multiple alignment of all the haplotypes [11, 14, 23, 5, 7]. In either approach, scalability is hampered by the encoding of all the haplotypes.

We suggest to look for a smaller set of representative haplotype sequences to make the above pan-genomic representations scalable.

Finding such set of representative haplotype sequences that retain the original contiguities as well as possible, is known as the founder sequence reconstruction problem [21]. In this problem, one seeks a set of $d$ founders such that the original $m$ haplotypes can be mapped with minimum amount of crossovers to the founders. Here a crossover means a position where one needs to jump from one founder to another to continue matching the content of the haplotype in question. Unfortunately, this problem in $\text{NP}$-hard even to approximate within a constant factor [15].

For founder reconstruction to be scalable to the pan-genomic setting, one would need an algorithm to be nearly linear to the input size. With this in mind, we study a relaxation of founder reconstruction that is known to be polynomial time solvable: Namely, when limiting all the crossovers to happen at the same locations, one obtains a minimum segmentation problem specific to founder reconstruction [21]. A dynamic programming algorithm given in [21] has complexity $O(n^2 m)$, where $m$ is the number of haplotypes and $n$ is the length of each of them.

In this paper, we improve the running time of solving the minimum segmentation problem of founder reconstruction to the optimal $O(mn)$ (linear in the input size).

We also implement the new algorithm, as well as a further heuristic that aims to minimize crossovers over the segment boundaries (yielded by the optimal solution to the minimum segmentation problem). In our experiments, we show that the approach is practical on human genome scale setting. Namely, we apply the implementation on a multiple alignment representing 5009 haplotypes of human chromosome 6, and the result is 130 founder sequences with the average distance of two crossovers being 9358 bases. Preserving such long contiguities in just 2.5% of the original input space is promising for the accuracy and scalability of the short read alignment and variant calling motivating our study.

The main technique behind the improvement is the use of positional Burrows–Wheeler transform (pBWT) [3], and more specifically its extension to larger alphabets [12]. While the original dynamic programming solution uses $O(nm)$ time to look for the best preceding segment boundary for each column of the input, we observe that at most $m$ values in pBWT determine segment boundaries where the number of distinct founder substrings change. Minimums on the already computed dynamic programming values between each such interesting consecutive segment boundaries give the requested result. However, it turns out that we can maintain the minimums directly in pBWT internal structures (with some modifications) and have to store only the last $L$ computed dynamic programming values, thus spending only $O(m + L)$ additional space, where $L$ is the input threshold on the length of each segment. The segmentation is then reconstructed by standard backtracking approach in $O(n)$ time using an array of length $n$.

2 Notation and Problem Statement

For a string $s = c_1c_2 \cdots c_n$, denote by $|s|$ its length $n$. We write $s[i]$ for the letter $c_i$ of $s$ and $s[i, j]$ for the substring $c_ic_{i+1}\cdots c_j$. An analogous notation is used for arrays. For any numbers $i$ and $j$, the set of integers $\{x \in \mathbb{Z}: i \leq x \leq j\}$ (possibly empty) is denoted by $[i, j]$. 
The input for our problem is the set \( R = \{ R_1, \ldots, R_m \} \) of strings of length \( n \), called recombinants. A set \( F = \{ F_1, \ldots, F_d \} \) of strings of length \( n \) is called a founder set of \( R \) if for each string \( R_i \in R \), there exists a partition \( P_i \) of the segment \([1, n]\) into disjoint subsegments such that, for each \([a, b] \in P_i \), the string \( R_i[a, b] \) is equal to \( F_j[a, b] \) for some \( j \in [1, d] \). The partition \( P_i \), together with the mapping of the segments \([a, b] \in P_i \) to substrings \( F_j[a, b] \) is called a parse of \( R_i \) in terms of \( F \), and a set of parses for all \( R_i \in R \) is called a parse of \( R \) in terms of \( F \). The integers \( a \) and \( b + 1 \), for \([a, b] \in P_i \), are called crossover points; thus, in particular, 1 and \( n + 1 \) are always crossover points.

It follows from the definition that, in practice, it makes sense to consider founder sets only for pre-aligned recombinants. Throughout the paper we implicitly assume that this is the case, although all our algorithms, clearly, work in the unaligned setting too but the produce results may hardly make any sense.

We consider the problem of finding a “good” founder set \( F \) and a “good” corresponding parse of \( R \) according to a reasonable measure of goodness. Ukkonen [21] pointed out that such measures may contradict each other: for instance, a minimum founder set obviously has size \( d = \max_{j \in [1, n]} |\{ R_1[j], \ldots, R_m[j]\}| \), but parses corresponding to such set may have unnaturally many crossover points; conversely, \( R \) is a founder set of itself and the only crossover points of its trivial parse are 1 and \( n + 1 \), but the size \( m \) of this founder set is in most cases unacceptably large. Following Ukkonen’s approach, we consider compromise parameterized solutions. The minimum founder set problem is, given a bound \( L \) and a set of recombinants \( R \), to find a smallest founder set \( F \) of \( R \) such that there exists a parse of \( R \) in terms of \( F \) in which the distance between any two crossover points is at least \( L \) (the crossover points may belong to parses of different recombinants, i.e., for \([a, b] \in P_i \) and \([a', b'] \in P_j \), where \( P_i \) and \( P_j \) are parses of \( R_i \) and \( R_j \), we have either \( a = a' \) or \(|a - a'| \geq L \)).

It is convenient to reformulate the problem in terms of segmentations of \( R \). A segment of \( R = \{ R_1, \ldots, R_m \} \) is a set \( R[j, k] = \{ R_i[j, k] : R_i \in R \} \). A segmentation of \( R \) is a collection \( S \) of disjoint segments that covers the whole \( R \), i.e., for any distinct \( R[j, k] \) and \( R[j', k'] \) from \( S \), \([j, k] \) and \([j', k'] \) do not intersect and, for each \( x \in [1, n] \), there is \( R[j, k] \) from \( S \) such that \( x \in [j, k] \). The minimum segmentation problem [21] is, given a bound \( L \) and a set of recombinants \( R \), to find a segmentation \( S \) of \( R \) such that \( \max\{|R[j, k]| : R[j, k] \in S\} \) is minimized and the length of each segment from \( S \) is at least \( L \); in other words, the problem is to compute

\[
\min_{S \in S_L} \max\{|R[j, k]| : R[j, k] \in S\},
\]

where \( S_L \) is the set of all segmentations in which all segments have length at least \( L \).

The minimum founder set problem and the minimum segmentation problem are, in a sense, equivalent: any founder set of \( R \) with segments of length at least \( L \) induces in an obvious way a founder set of size \( \max\{|R[j, k]| : R[j, k] \in S\} \) and a parse in which all crossover points are located at segment boundaries (and, hence, at distance at least \( L \) from each other); conversely, if \( F \) is a founder set of \( R \) and \( \{j_1, \ldots, j_q\} \) is the sorted set of all crossover points in a parse of \( R \) such that \( j_q - j_{q-1} \geq L \) for \( q \in [2, p] \), then \( S = \{ R[j_{q-1}, j_q-1] : q \in [2, p] \} \) is a segmentation of \( R \) with segments of length at least \( L \) and \( \max\{|R[j, k]| : R[j, k] \in S\} \leq |F| \).

Our main result is an algorithm that solves the minimum segmentation problem in the optimal \( O(mn) \) time. The solution normally does not uniquely define a founder set of \( R \); for instance, if the built segmentation of \( R = \{ baaaa, baab, babab \} \) is \( S = \{ R[1, 1], R[2, 3], R[4, 5] \} \), then the possible founder sets induced by \( S \) are \( F_1 = \{ baaba, babaa \} \) and \( F_2 = \{ baaca, babab \} \).

In other words, to construct a founder set, one concatenates fragments of recombinants corresponding to the found segments in a certain order. We return to this ordering problem in Sect. 4 and now focus on the details of the segmentation problem.
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Hereafter, we assume that the input alphabet Σ is the set $[0, |Σ| - 1]$ of size $O(m)$, which is a natural assumption considering that the typical alphabet size is 4 in our problem. It is sometimes convenient to view the set $R = \{ R_1, \ldots, R_m \}$ as a matrix with $m$ rows and $n$ columns. We say that an algorithm processing the recombinants $R$ is streaming if it reads the input from left to right “columnwise”, for each $k$ from 1 to $n$, and outputs an answer for each set of recombinants $\{ R_1[1,k], \ldots, R_m[1,k] \}$ immediately after reading the “column” $\{ R_1[k], \ldots, R_m[k] \}$. The main result of the paper is the following theorem.

**Theorem 1.** Given a bound $L$ and recombinants $R = \{ R_1, \ldots, R_m \}$, each having length $n$, there is an algorithm that computes (1) in a streaming fashion in the optimal $O(mn)$ time and $O(m + L)$ space. Using an additional array of length $n$, one can also find in $O(n)$ time a segmentation on which (1) is attained, thus solving the minimum segmentation problem.

### 3 Minimum Segmentation Problem

Given a bound $L$ and a set of recombinants $R = \{ R_1, \ldots, R_m \}$ each of which has length $n$, Ukkonen [21] proposed a dynamic programming algorithm that solves the minimum segmentation problem in $O(mn^2)$ time based on the following recurrence relation:

$$M(k) = \begin{cases} +\infty & \text{if } k < L, \\ |R[1,k]| & \text{if } L \leq k < 2L, \\ \min_{0 \leq j \leq k-L} \max \{ M(j), |R[j+1,k]| \} & \text{if } k \geq 2L. \end{cases} \quad (2)$$

It is obvious that $M(n)$ is equal to the solution (1); the segmentation itself can be reconstructed by “backtracking” in a standard way (see [21]). We build on the same approach.

For a given $k \in [1,n]$, denote by $j_{k,1}, \ldots, j_{k,r_k}$ the sequence of all positions $j \in [1, k - L]$ in which the value of $|R[j,k]|$ changes, i.e., $1 \leq j_{k,1} < \cdots < j_{k,r_k} \leq k - L$ and $|R[j_{k,h},k]| \neq |R[j_{k,h+1},k]|$ for $h \in [1,r_k]$. We complement this sequence with $j_{k,0} = 0$ and $j_{k,r_k+1} = k - L + 1$, so that $j_{k,0}, \ldots, j_{k,r_k+1}$ can be interpreted as a splitting of the range $[0, k - L]$ into segments in which the value $|R[j,k]|$ stays the same: namely, for $h \in [0, r_k]$, one has $|R[j,k]| = |R[j+h,k]|$ provided $j_k \leq j < j_{k,h+1}$. Hence, $\min_{j_k \leq h < j_{k,h+1}} \max \{ M(j), |R[j+1,k]| \} = \max \{ |R[j_k+h+1,k]|, \min_{j_k \leq j < j_{k,h+1}} M(j) \}$ and, therefore, (2) can be rewritten as follows:

$$M(k) = \begin{cases} +\infty & \text{if } k < L, \\ |R[1,k]| & \text{if } L \leq k < 2L, \\ \min_{0 \leq h \leq r_k} \max \{ |R[j_k+h+1,k]|, \min_{j_k \leq j < j_{k,h+1}} M(j) \} & \text{if } k \geq 2L. \end{cases} \quad (3)$$

Our crucial observation is that, for $k \in [1,n]$ and $j \in [1,k]$, one has $|R[j+1,k]| \leq |R[j,k]| \leq m$. Therefore, $m \geq |R[j_k,k]| > \cdots > |R[j_{k,r_k+1},k]| \geq 1$ and $r_k < m$. Hence, $M(k)$ can be computed in $O(m)$ time using (3), provided one has the following components:

(i) the numbers $|R[j_k+h+1,k]|$, for $h \in [0, r_k]$;
(ii) the values $\min \{ M(j) : j_k \leq j < j_{k+1} \}$, for $h \in [0, r_k]$.

In the remaining part of the section, we describe a streaming algorithm that reads the strings $\{ R_1, \ldots, R_m \}$ “columnwise” from left to right and computes the components (i) and (ii) immediately after reading each “column” $\{ R_1[k], \ldots, R_m[k] \}$, for $k \in [1,n]$, and all in $O(mn)$ total time and $O(m + L)$ space.

To reconstruct a segmentation corresponding to the found solution $M(n)$, we build along with the values $M(k)$ an array of size $n$ whose $k$th element, for each $k \in [1,n]$, stores $0$ if $M(k) = |R[1,k]|$, and stores a number $j \in [1, k-L]$ such that $M(k) = \max \{ M(j), |R[j+1,k]| \)$.
otherwise; then, the segmentation can be reconstructed from the array in an obvious way in $O(n)$ time. In order to maintain the array, our algorithm computes, for each $k \in [1,n]$, along with the values $\min\{M(j) : j_k, h \leq j < j_{k,h+1}\}$, for $h \in [0,r_k]$, positions $j$ on which these minima are attained (see below). Further details are straightforward and, thence, omitted.

### 3.1 Positional Burrows–Wheeler Transform

Let us fix $k \in [1,n]$. Throughout this subsection, the string $R_i[k]R_i[k-1] \ldots R_i[1]$, which is the reversal of $R_i[1,k]$, is denoted by $R'_i[k]$, for $i \in [1,m]$. Given a set of recombinants $\mathcal{R} = \{R_1, \ldots, R_m\}$ each of which has length $n$, a positional Burrows–Wheeler transform (pBWT), as defined by Durbin [3], is a pair of integer arrays $a_k[1,m]$ and $d_k[1,m]$ such that:

1. $a_k[1,m]$ is a permutation of $[1,m]$ such that $R'_a[i][1,k] \leq \cdots \leq R'_a[m][1,k]$ lexicographically;
2. $d_k[i]$, for $i \in [1,m]$, is an integer such that $R_{a_k[i]}[d_k[i], k]$ is the longest common suffix of $R_{a_k[i]}[1,k]$ and $R_{a_k[i-1]}[1,k]$, and $d_k[i] = k + 1$ if either this suffix is empty or $i = 1$.

**Example 2.** Consider the following example, where $m = 6$, $k = 7$, and $\Sigma = \{a,c,t\}$. It is easy to see that the pBWT implicitly encodes the trie depicted in the right part of Figure 1, and such interpretation drives the intuition behind this structure: The trie represents the reversed sequences $R_i[1,k]$, $\ldots$, $R_i[k-1]$ (i.e., read from right to left) in lexicographic order. Leaves (values $a_k$) store the corresponding input indices. The branches correspond to values $d_k$ (the distance from the root subtracted from $k + 1$). Our main algorithm in this paper makes implicitly a sweep-line over the trie stopping at the branching positions.

Durbin [3] showed that $a_k$ and $d_k$ can be computed from $a_{k-1}$ and $d_{k-1}$ in $O(m)$ time on the binary alphabet. Mäkinen and Norri [12] further generalized the construction for integer alphabets of size $O(m)$, as in our case. For the sake of completeness, we describe in this subsection the solution from [12] (see Figure 2a), which serves then as a basis for our main algorithm. We also present a modification of this solution (see Figure 2b), which, albeit seems to be slightly inferior in theory (we could prove only $O(m \log |\Sigma|)$ time upper bound), showed better performance in practice and thus, as we believe, is interesting by itself.

**Lemma 3.** The arrays $a_k[1,m]$ and $d_k[1,m]$ can be computed from $a_{k-1}[1,m]$ and $d_{k-1}[1,m]$ in $O(m)$ time, assuming the input alphabet is $[0,|\Sigma|-1]$ with $|\Sigma| = O(m)$.

**Proof.** Given $a_{k-1}$ and $d_{k-1}$, we are to show that the algorithm from Figure 2a correctly computes $a_k$ and $d_k$. Since, for any $i,j \in [1,m]$, we have $R'_{i,k} \leq R'_{j,k}$ if and only if $R_i[k] < R_j[k]$, or $R_i[k] = R_j[k]$ and $R'_{i,k-1} \leq R'_{j,k-1}$ lexicographically, it is easy to see that the array $a_k$ can be deduced from $a_{k-1}$ by radix sorting the sequence of pairs $\{(R_{a_{k-1}[i]}[k], R'_{a_{k-1}[i]}[k-1])\}_{i=1}^m$. Further, since, by definition of $a_{k-1}$, the second components of the pairs are already in a sorted order, it remains to sort the first components by the counting sort. Accordingly, in
zero initialize \( C[0,|\Sigma|] \) and \( P[0,|\Sigma| - 1] \)

for \( i \leftarrow 1 \) to \( m \) do

\( C[R_i[k] + 1] \leftarrow C[R_i[k] + 1] + 1; \)

for \( i \leftarrow 1 \) to \( |\Sigma| - 1 \) do

\( C[i] \leftarrow C[i] + C[i-1]; \)

for \( i \leftarrow 1 \) to \( m \) do

\( b \leftarrow R_{a_{k-1}[i]}[k]; \)

\( C[b] \leftarrow C[b] + 1; \)
\( a_k[C[b]] \leftarrow a_{k-1}[i]; \)

if \( P[b] = 0 \) then

\( d_k[C[b]] \leftarrow k + 1; \)

else

\( d_k[C[b]] \leftarrow \max\{d_{k-1}[\ell]: P'[\ell] < \ell \leq i\}; \)

\( P[b] \leftarrow i; \)

end if

end for

end for

end for

Figure 2a, the first loop counts occurrences of letters in the sequence \( \{R_i[k]\}_{i=1}^m \) using an auxiliary array \( C[0,|\Sigma|] \); as is standard in the counting sort, the second loop modifies the array \( C \) so that, for each letter \( b \in [0,|\Sigma|-1], C[b] + 1 \) is the first index of the ”bucket” that will contain all \( a_{k-1}[i] \) such that \( R_{a_{k-1}[i]}[k] = b \); finally, the third loop fills the buckets incrementing the indices \( C[b] \leftarrow C[b] + 1 \), for \( b = R_{a_{k-1}[i]}[k] \), and performing the assignments \( a_k[C[b]] \leftarrow a_{k-1}[i] \), for \( i = 1, \ldots, m \). Thus, the array \( a_k \) is computed correctly. All is done in \( O(m + |\Sigma|) \) time, which is \( O(m) \) since the input alphabet is \( [0,|\Sigma|-1] \) and \( |\Sigma| = O(m) \).

The last three lines of the algorithm are responsible for computing \( d_k \). Denote the length of the longest common prefix of any strings \( s_1 \) and \( s_2 \) by \( \text{LCP}(s_1, s_2) \). The computation of \( d_k \) relies on the following well-known fact: given a sequence of strings \( s_1, \ldots, s_r \), such that \( s_1 \leq \cdots \leq s_r \) lexicographically, one has \( \text{LCP}(s_1, s_r) = \min\{\text{LCP}(s_i, s_j): 1 \leq i \leq r\} \). Suppose that the last loop of the algorithm, which iterates through all \( i \) from 1 to \( m \), assigns \( a_k[i'] \leftarrow a_{k-1}[i] \), for a given \( i \in [1,m] \) and some \( i' = C[b] \). Let \( j \) be the maximum integer such that \( j < i \) and \( R_{a_{k-1}[j]}[k] = R_{a_{k-1}[i]}[k] \) (if any). The definition of \( a_k \) implies that \( a_k[i' \leq j] \equiv a_{k-1}[j] \) if such \( j \) exists. Hence, \( \text{LCP}(R_{a_k[i' \leq j]}[k], R_{a_k[i']}[k]) = 1 + \min\{\text{LCP}(R_{a_k[i' \leq j]}[\ell-1], k-1), R_{a_k[i']}[\ell-1], k-1) : j < \ell \leq i\} \) if such number \( j \) does exist, and \( \text{LCP}(R_{a_k[i' \leq j]}[k], R_{a_k[i']}[k]) = 0 \) otherwise. Therefore, since \( d_k[i'] \) equals \( k + 1 - \text{LCP}(R_{a_k[i']}[k], R_{a_k[i']}[k]) \), we have either \( d_k[i'] = \max\{d_{k-1}[\ell] : j < \ell \leq i\} \) or \( d_k[i'] = k + 1 \) according to whether the required \( j \) exists. To find \( j \), we simply maintain an auxiliary array \( P[0,|\Sigma|-1] \) such that on the \( i \)th loop iteration, for any letter \( b \in [0,|\Sigma|-1], P[b] \) stores the position of the last seen \( b \) in the sequence \( R_{a_{k-1}[i]}[k], R_{a_{k-2}[2][k], \ldots, R_{a_{k-1}[i]}[k] \), or \( P[b] = 0 \) if \( b \) occurs for the first time. Thus, \( d_k \) is computed correctly.

In order to calculate the maximums \( \max\{d_{k-1}[\ell] : P'[\ell] \leq \ell \leq i\} \) in \( O(1) \) time, we build a range maximum query (RMQ) data structure on the array \( d_{k-1}[1,m] \) in \( O(m) \) time (e.g., see [6]). Therefore, the running time of the algorithm from Figure 2a is \( O(m) \).

In practice the bottleneck of the algorithm is the RMQ data structure, which, although answers queries in \( O(1) \) time, has a sensible constant under the big-O in the construction time. We could naively compute the maximums by scanning the ranges \( d_{k-1}[P'[b] + 1, i] \) from
left to right but such algorithm works in quadratic time since same ranges of \( d_{k - 1} \) might be processed many times in the worst case. Our key idea is to store the work done by a simple scanning algorithm to reuse it in future queries. We store this information right in the arrays \( a_{k - 1} \) and \( d_{k - 1} \) rewriting them; in particular, since \( a_{k - 1} \) is accessed sequentially from left to right in the last loop, the range \( a_{k - 1}[i] \) is free to use after the \( i \)th iteration.

More precisely, after the \( i \)th iteration of the last loop, the subarrays \( a_{k - 1}[1, i] \) and \( d_{k - 1}[1, i] \) are modified so that the following invariant holds: for any \( j \in [1, i] \), \( j < a_{k - 1}[j] \leq i + 1 \) and \( d_{k - 1}[j] = \max\{d'_{k - 1}[\ell] : j \leq \ell < a_{k - 1}[j]\} \), where \( a_{k - 1} \) denotes the original array \( d_{k - 1} \) before modifications; note that the invariant holds if one simply puts \( a_{k - 1}[j] = j + 1 \) without altering \( d_{k - 1}[j] \). Then, to compute \( \max\{d'_{k - 1}[\ell] : j \leq \ell \leq i\} \), we do not have to scan all elements but can “jump” through the chain \( j, a_{k - 1}[j], a_{k - 1}[a_{k - 1}[j]], \ldots, i \) and use maximums precomputed in \( d_{k - 1}[j], d_{k - 1}[a_{k - 1}[j]], d_{k - 1}[a_{k - 1}[a_{k - 1}[j]]], \ldots, d_{k - 1}[i] \); after this, we redirect the “jump pointers” in \( a_{k - 1} \) to \( i + 1 \) and update the maximums in \( d_{k - 1} \) accordingly. This idea is implemented in Figure 2b. Notice the new line \( a_{k - 1}[i] \leftarrow i + 1 \) in the main loop (it is commented), which erases \( a_{k - 1}[i] \) and makes it a part of the “jump table”. The correctness of the algorithm is clear. But it is not immediate even that the algorithm works in \( O(m \log m) \) time. The next lemma states that the bound is actually even better, \( O(m \log |\Sigma|) \). The proof of the lemma is given in Appendix.

**Lemma 4.** The algorithm from Figure 2b computes the arrays \( a_k[1, m] \) and \( d_k[1, m] \) from \( a_{k - 1}[1, m] \) and \( d_{k - 1}[1, m] \) in \( O(m \log |\Sigma|) \) time, assuming the input alphabet is \([0, |\Sigma| - 1]\) with \(|\Sigma| = O(m)\).

### 3.2 Modification of the pBWT

We are to modify the basic pBWT construction algorithm in order to compute the sequence \( j_{k,1}, \ldots, j_{k, r_k} \) of all positions \( j \in [1, k - L] \) in which \( |R[j, k]| \neq |R[j + 1, k]| \), and to calculate the numbers \( |R[j_{k, h+1}, k]| \) and \( \min(M(j) : j_{k, h} \leq j < j_{k, h+1}) \) for \( h \in [0, r_k] \) (assuming \( j_{k, 0} = 0 \) and \( j_{k, r_k+1} = k - L + 1 \)); see the beginning of the section. As it follows from (3), these numbers are sufficient to calculate \( M(k) \), as defined in (2) and (3), in \( O(m) \) time. The following lemma reveals relations between the sequence \( j_{k,1}, \ldots, j_{k, r_k} \) and the array \( d_k \).

**Lemma 5.** Consider recombinants \( R = \{R_1, \ldots, R_m\} \), each having length \( n \). For \( k \in [1, n] \) and \( j \in [1, k - 1] \), one has \( |R[j, k]| \neq |R[j + 1, k]| \) iff \( j = d_k[i] - 1 \) for some \( i \in [1, m] \).

**Proof.** Suppose that \( |R[j, k]| \neq |R[j + 1, k]| \). It is easy to see that \( |R[j, k]| > |R[j + 1, k]| \), which implies that there are two indices \( h \) and \( h' \) such that \( R_h[j + 1, k] = R_{h'}[j + 1, k] \) and \( R_h[j] \neq R_{h'}[j] \). Denote by \( a_k^{-1}[h] \) the number \( x \) such that \( a_k[x] = h \). Without loss of generality, assume that \( a_k^{-1}[h] < a_k^{-1}[h'] \). Then, there exists \( i \in [a_k^{-1}[h] + 1, a_k^{-1}[h']] \) such that \( R_{a_k[i-1]}[j + 1, k] = R_{a_k[i]}[j + 1, k] \) and \( R_{a_k[i-1]}[j] \neq R_{a_k[i]}[j] \). Hence, \( d_k[i] = j + 1 \).

Suppose now that \( j \in [1, k - 1] \) and \( j = d_k[i] - 1 \), for some \( i \in [1, m] \). Since \( j < k \) and \( d_k[1] = k + 1 \), we have \( i > 1 \). Then, by definition of \( d_k \), \( R_{a_k[i-1]}[j + 1, k] = R_{a_k[i]}[j + 1, k] \) and \( R_{a_k[i-1]}[j] \neq R_{a_k[i]}[j] \), i.e., \( R_{a_k[i]}[j + 1, k] \) can be “extended” to the left in two different ways, thus producing two distinct strings in the set \( R[j, k] \). Therefore, \( |R[j, k]| > |R[j + 1, k]| \).
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\[ t_k[1,r]: \text{for } j \in [1,r], t_k[j] \text{ is equal to the number of times } s_k[j] \text{ occurs in } d_k[1,m]; \]

\[ u_k[1,r]: \text{for } j \in [1,r], u_k[j] = \min\{M'(\ell): s_k[j-1]-1 \leq \ell < s_k[j]-1\}, \text{assuming } s_k[0] = 1. \]

**Example 6.** In Example 2, where \( m = 6, k = 7, \text{ and } \Sigma = \{a,c,t\} \), we have \( r = 4, \)
\( s_k = [3,5,7,8], t_k = [2,1,1,2], \) \( e_k = [4,2,1,3,1]. \) It is easy to see that the array \( s_k \) marks positions of the branching nodes in the trie from Figure 1 in the increasing order (in the special case \( s_k[1] = 1, s_k[1] \) does not mark any such node). The arrays \( s_k \) and \( e_k \) together emulate \( d_k. \) The array \( t_k \) will be used below to calculate some numbers \( |R[j,k]| \) required to compute \( M(k). \) Further, suppose that \( L = 3, \) so that \( k - L = 4. \) Then, \( u_k[1] = M(1), u_k[2] = \min\{M(2), M(3)\}, u_k[3] = \min\{M(4), M'(5)\} = M(4) \text{ since } M'(5) = +\infty, \text{ and } u_k[4] = M'(6) = +\infty. \) The use of \( u_k \) is discussed in the sequel.

For convenience, let us recall Equation (3) defined in the beginning of this section:

\[ M(k) = \begin{cases} +\infty & \text{if } k < L, \\ |R[1,k]| & \text{if } L \leq k < 2L, \\ \min_{0 \leq h \leq r} \max\{|R[j,h+1,k]|, \min_{j,h,2 \leq j < k,h+1} M(j)\} & \text{if } k \geq 2L, \end{cases} \tag{3 revisited} \]

where \( j_{k,0} = 0, j_{k,r_k+1} = k-L+1, \) and \( j_{k,1}, \ldots, j_{k,r_k} \) is the increasing sequence of all positions \( j \in [1,k-L] \) in which \( |R[j,k]| \neq |R[j+1,k]|. \) In order to compute \( M(k) \), one has to find the minima \( \min_{j,k,2 \leq j \leq k,h+1} M(j) \) and calculate \( |R[j,k]| \). As it follows from Lemma 5 and the definition of \( s_k \), all positions \( j \in [1,k-1] \) in which \( |R[j,k]| \neq |R[j+1,k]| \) are represented by the numbers \( s_k[i] - 1 \) such that \( 1 < s_k[i] \leq k \) (in the increasing order); hence, the sequence \( j_{k,1}, \ldots, j_{k,r_k} \) corresponds to either \( s_k[1] - 1, \ldots, s_k[r_k]-1 \) or \( s_k[2] - 1, \ldots, s_k[r_k+1]-1, \) depending on whether \( s_k[1] = 1 \). Then, the minima \( \min_{j,k,2 \leq j \leq k,h+1} M(j) \) are stored in the corresponding elements of \( u_k \) (assuming \( s_k[0] = 1): u_k[i] = \min\{M' (\ell): s_k[i-1]-1 \leq \ell < s_k[i]-1\} = \min\{M(\ell): s_k[i-1]-1 \leq \ell < \min\{s_k[i]-1,k-L+1\}\} = \min_{j,k,2 \leq j \leq k,h+1} M(j), \) provided \( s_k[i-1]-1 = j_{k,h}. \) It is clear that \( u_k[i] \neq +\infty \) only if the segment \( [s_k[i-1]-1, s_k[i]-2] \) intersects the range \( [1,k-L] \) and, thus, corresponds to a segment \( [j_{k,h}, j_{k,h+1}-1], \) for \( h \in [0,r_k]. \) Therefore, since \( M'(\ell) = +\infty \) for \( \ell < 1 \) and \( \ell > k-L \) and, thus, such values \( M'(\ell) \) do not affect, in a sense, the minima stored in \( u_k, \) one can rewrite (3) as follows:

\[ M(k) = \begin{cases} +\infty & \text{if } k < L, \\ |R[1,k]| & \text{if } L \leq k < 2L, \\ \min_{1 \leq j \leq |s_k|} \max\{|R[s_k[j]-1,k]|, u_k[j]\} & \text{if } k \geq 2L. \end{cases} \tag{4} \]

It remains to compute the numbers \( |R[s_k[j]-1,k]|, \) for \( j \in [1,|s_k|]. \)

**Lemma 7.** Consider a set of recombinants \( R = \{R_1, \ldots, R_m\}, \) each of which has length \( n. \)

For \( k \in [1,n] \) and \( j \in [1,|s_k|], \) one has \( |R[s_k[j]-1,k]| = t_k[j] + t_k[j+1] + \cdots + t_k[|t_k|]. \)

**Proof.** Denote \( \ell = k-s_k[j]+1, \) so that \( |R[s_k[j]-1,k]| = |R[k-\ell,k]|. \) Suppose that \( \ell = 0. \) Note that \( R_{a_k[i]}[k] \leq \cdots \leq R_{a_k[n]}[k]. \) Since \( d_k[i] = k+1 \) iff either \( i = 1 \) or \( R_{a_k[i-1]}[k] \neq R_{a_k[i]}[k], \) it is easy to see that \( |R[k,\ell]|, \) the number of distinct letters \( R_{k,l} \), is equal to the number of time \( k+1 = s_k[i] \) occurs in \( d_k, \) i.e., \( t_k[|t_k|]. \)

Suppose that \( \ell > 0. \) It suffices to show that \( |R[k-\ell,k]| - |R[k-\ell+1,k]| = t_k[j]. \) For \( i \in [1,m], \) denote by \( R_{i}^* \) the string \( R_{i}[k][k-1] \cdots R_{i}[k-\ell]. \) Fix \( w \in R[k-\ell+1,k]. \) Since \( R_{a_k[i]} \leq \cdots \leq R_{a_k[n]} \) lexicographically, there are numbers \( h \) and \( h' \) such that \( R_{a_k[i]}[k-\ell+1,k] = w \) iff \( i \in [h,h'). \) Further, we have \( R_{a_k[i]}[k-\ell] \leq R_{a_k[h+1]}[k-\ell] \leq \cdots \leq R_{a_k[n]}[k-\ell]. \)
Algorithm 1 Computing $e_i$, $s_k$, $t_k$, $u_k$, $a_k$ from $e_{k-1}$, $s_{k-1}$, $t_{k-1}$, $u_{k-1}$, $a_{k-1}$.

1: copy $s_{k-1}$ into $s_k$ and add the element $k + 1$ to the end of $s_k$, thus incrementing $|s_k|$;
2: copy $u_{k-1}$ into $u_k$ and add the element $M'(k - 1)$ to the end of $u_k$, thus incrementing $|u_k|$;
3: zero initialize $C[0, |\Sigma|]$, $P[0, |\Sigma| - 1]$, and $t_k[1, |s_k|]$;
4: for $i \leftarrow 1$ to $m$ do $C[R[i][k] + 1] \leftarrow C[R[i][k]] + 1$;
5: for $i \leftarrow 1$ to $|\Sigma| - 1$ do $C[i] \leftarrow C[i] + C[i - 1]$;
6: for $i \leftarrow 1$ to $m$ do
7: \hspace{1em} $b \leftarrow R_{a_k[i][k]}[k]$;
8: \hspace{1em} $C[b] \leftarrow C[b] + 1$;
9: \hspace{1em} $a_k[C[b]] \leftarrow a_k[i][k]$;
10: \hspace{1em} if $P[b] = 0$ then $e_k[C[b]] \leftarrow |s_k|$;
11: \hspace{1em} else $e_k[C[b]] \leftarrow \max\{e_k[\ell], P[b] < \ell \leq i\}$
12: \hspace{1em} $P[b] \leftarrow i$;
13: for $i \leftarrow 1$ to $m$ do $t_k[e_k[i]] \leftarrow t_k[e_k[i]] + 1$;
14: $j \leftarrow 1$;
15: add a new “dummy” element $\infty$ to the end of $u_k$ and $u_{k-1}$;
16: for $i \leftarrow 1$ to $|s_k|$ do
17: \hspace{1em} $u_k[j] \leftarrow \min\{u_k[j], u_{k-1}[i]\}$;
18: \hspace{1em} if $t_k[i] \neq 0$ then
19: \hspace{1em} \hspace{1em} $tmp[i] \leftarrow j$;
20: \hspace{1em} \hspace{1em} $s_k[j] \leftarrow s_k[i], t_k[j] \leftarrow t_k[i], u_k[j + 1] \leftarrow u_k[i + 1]$;
21: \hspace{1em} \hspace{1em} if $s_k[j - 1] > k - L$ and $(j = 1$ or $s_k[j - 1] - 1 \leq k - L)$ then $u_k[j] \leftarrow \min\{u_k[j], M(k - L)\}$;
22: \hspace{1em} \hspace{1em} $j \leftarrow j + 1$;
23: shrink $s_k$, $t_k$, and $u_k$ to $j - 1$ elements, so that $|s_k| = |t_k| = |u_k| = j - 1$;
24: for $i \leftarrow 1$ to $m$ do $e_k[i] \leftarrow tmp[e_k[i]]$;

Thus, by definition of $d_k$, for $i \in [h + 1, h']$, we have $R_{a_k[i-1][k-\ell]} \neq R_{a_k[i][k-\ell]}$ iff $d_k[i] = k - \ell + 1 = s_k[j]$. Note that $d_k[h] > s_k[j]$. Therefore, the number of strings $R[k-\ell, k]$ from $\mathcal{R}[k-\ell, k]$ having suffix $\sigma$ is equal to one plus the number of integers $s_k[j]$ in the range $d_k[h, h']$, which implies $|\mathcal{R}[k-\ell, k]| - |\mathcal{R}[k-\ell + 1, k]| = t_k[j]$.

By (4) and Lemma 7, one can calculate $M(k)$ in $O(m)$ time using the arrays $t_k$ and $u_k$.

It remains to describe how we maintain $a_k, e_k, s_k, t_k, u_k$.

\begin{lemma}
The arrays $a_k, e_k, s_k, t_k, u_k$ can be computed from $a_{k-1}, e_{k-1}, s_{k-1}, t_{k-1}, u_{k-1}$ and from the numbers $M(k - L)$ and $M(k - 1)$ in $O(m)$ time, assuming the input alphabet is $\Sigma$.
\end{lemma}

\begin{proof}
Let us analyze Algorithm 1 that computes $a_k, e_k, s_k, t_k, u_k$. By definition, $d_{k-1}[i] = s_{k-1}[e_{k-1}[i]]$ for $i \in [1, m]$. The first line of the algorithm initializes $s_k$ so that $d_{k-1}[i] = s_k[e_{k-1}[i]]$ for $i \in [1, m]$, and $s_k[|s_k|] = k + 1$. Since after this initialization $s_k$, obviously, is in the sorted order, one has, for $i, j \in [1, m]$, $e_{k-1}[i] \leq e_{k-1}[j]$ iff $d_{k-1}[i] \leq d_{k-1}[j]$ and, therefore, for $\ell \in [i, j]$, one has $d_{k-1}[\ell] = \max\{d_{k-1}[\ell'] : i \leq \ell' \leq j\}$ if $e_{k-1}[\ell] = \max\{e_{k-1}[\ell'] : i \leq \ell' \leq j\}$.

Based on this observation, we fill $e_k$ in lines 3–12 so that $d_k[i] = s_k[e_k[i]]$, for $i \in [1, m]$, using exactly the same algorithm as in Figure 2a, where $d_k$ is computed, but instead of the assignment $d_k[C[b]] \leftarrow k + 1$, we have $e_k[C[b]] \leftarrow |s_k|$ since $s_k[|s_k|] = k + 1$. Here we also compute $a_k$ in the same way as in Figure 2a.

The loop in line 13 fills $t_k$ so that, for $i \in [1, |s_k|]$, $t_k[i]$ is the number of occurrences of the integer $i$ in $e_k$ ($t_k$ was zero initialized in line 3). Since, for $i \in [1, m]$, we have $d_k[i] = s_k[e_k[i]]$ at this point, $t_k[i]$ is also the number of occurrences of the integer $s_k[i]$ in $d_k[1, m]$.

By (4) and Lemma 7, one can calculate $M(k)$ in $O(m)$ time using the arrays $t_k$ and $u_k$.
By definition, $s_k$ must contain only elements from $d_k$, but this is not necessarily the case in line 14. In order to fix $s_k$ and $t_k$, we simply have to remove all elements $s_k[i]$ for which $t_k[i] = 0$, moving all remaining elements of $s_k$ and non-zero elements of $t_k$ to the left accordingly. Suppose that, for some $n$ and $i$, we have $e_k[n] = i$ and the number $s_k[i]$ is moved to $s_k[j]$, for some $j < i$, as we fix $s_k$. Then, $e_k[n]$ must become $j$. We utilize an additional temporary array $tmp[1, |s_k|]$ to fix $e_k$. The loop in lines 16–22 fixes $s_k$ and $t_k$ in an obvious way: once $s_k[i]$ is moved to $s_k[j]$ during this process, we assign $tmp[i] = j$. Then, $s_k$, $t_k$, $u_k$ ($u_k$ is discussed below) are resized in line 23, and the loop in line 24 fixes $e_k$ using $tmp$.

Recall that $[s_k[j - 1] - 1, s_k[j] - 2]$, for $j \in [1, |s_k|]$, is a system of disjoint segments covering $[0, k-1]$ (assuming $s_k[0] = 1$). It is now easy to see that this system is obtained from the system $[s_k-1[j - 1] - 1, s_k-1[j] - 2]$, with $j \in [1, |s_k-1|]$ (assuming $s_k-1[0] = 1$), by adding the new segment $[k - 1, k-1]$ and joining some segments together. The second line of the algorithm copies $u_{k-1}$ into $u_k$ and adds $M'(k-1)$ to the end of $u_k$, so that, for $j \in [1, |u_{k-1}|]$, $u_k[j]$ is equal to the minimum of $M'(\ell)$ for all $\ell$ from the segment $[s_k-1[j - 1] - 1, s_k-1[j] - 2]$ and $u_k[|u_{k-1}| + 1] = M'(k-1)$ is the minimum in the segment $[k - 1, k-1]$. (This is not completely correct since $M'$ has changed as $k$ was increased; namely, $M'(k - L)$ was equal to $+\infty$ but now is equal to $M(k - L)$.) As we join segments removing some elements from $s_k$ in the loop 16–22, the array $u_k$ must be fixed accordingly: if $[s_k[j - 1] - 1, s_k[j] - 2]$ is obtained by joining $[s_{k-1}[h - 1] - 1, s_{k-1}[h] - 2]$, for $j' \leq h \leq j''$, then $u_k[j] = \min\{u_k[h]: j' \leq h \leq j''\}$. We perform such fixes in line 17, accumulating the latter minimum. We start accumulating a new minimum in line 20, assigning $u_k[j + 1] \leftarrow u_{k-1}[i + 1]$. If at this point the ready minimum accumulated in $u_{k-1}$ corresponds to a segment containing the position $k - L$, we have to fix $u_k$ taking into account the new value $M'(k - L) = M(k - L)$; we do this in line 21. To avoid accessing out of range elements in $u_k$ and $u_{k-1}$ in line 20, we add a “dummy” element in, respectively, $u_k$ and $u_{k-1}$ in line 15.

Besides all the arrays of length $m$, the algorithm from Lemma 8 also requires access to $M(k - L)$ and, possibly, to $M(k - 1)$. During the computation of $M(k)$ for $k \in [1, n]$, we maintain the last $L$ calculated numbers $M(k - 1), M(k - 2), \ldots, M(k - L)$ in a circular array, so that the overall required space is $O(m + L)$; when $k$ is incremented, the array is modified in $O(1)$ time in an obvious way. Thus, Lemma 8 implies Theorem 1.

If, as in our case, one does not need $s_k, t_k, u_k$ for all $k$, the arrays $s_k, t_k, u_k$ can be modified in-place, i.e., $s_k, t_k, u_k$ can be considered as aliases for $s_{k-1}, t_{k-1}, u_{k-1}$, and yet the algorithm remains correct. Thus, we really need only 7 arrays in total: $a_k, a_{k-1}, e_k, e_{k-1}, s, t, u$, where $s, t, u$ serve as $s_k, t_k, u_k$ and the array $tmp$ can be organized in place of $a_{k-1}$ or $e_{k-1}$. It is easy to maintain along with each value $u_k[j]$ a corresponding position $\ell$ such that $u_k[j] = M'(\ell)$; these positions can be used then to restore the found segmentation of $R$ using backtracking (see the beginning of the section). To compute $e_k$, instead of using an RMQ data structure, one can adapt in an obvious way the algorithm from Figure 2b rewriting the arrays $a_{k-1}$ and $e_{k-1}$ during the computation, which is faster in practice but theoretically takes $O(m \log \sigma)$ time by Lemma 4. We do not discuss further details as they are straightforward.

## 4 Implementation

We implemented the segmentation algorithm using Lemma 4 to build the data structures, and thus the overall time complexity of the implemented approach is $O(mn \log \sigma)$. The implementation outputs for each segment the distinct founder sequence fragments, and associates to each fragment the set of haplotypes containing that fragment as a substring.
at that location (these are easily deduced given the segmentation and the positional BWT structures). As discussed earlier, to obtain full founder sequences, one needs to concatenate these fragments in some order. If each segment has exactly the same amount of fragments, there is a way of finding an optimal concatenation minimizing the number of crossovers [21]: For any two consecutive segments, form a bipartite graph with fragments as nodes and edges corresponding to plausible concatenations. The cost of an edge is the symmetric difference of the sets associated with the fragments. Minimum cost perfect matching then gives an optimal concatenation order. Each consecutive pair can be solved independently, and founder sequences can be extracted through the paths formed by matches edges. However, not all segments may contain the maximum amount of distinct fragments; we conjecture the ordering problem becomes hard in this case (due to the local matchings being no longer independent). There are many possible heuristic ways to alleviate this issue, among which we opted to preprocess the segments to have the same amount of fragments; we duplicated the fragments greedily according to the sizes of the associated sets. Then we used the matching approach described above. In the upcoming extended version of this paper, we plan to study an alternative approach that provides an approximation guarantee.

To test the implementation of our algorithm, we generated a multiple alignment of haplotype sequences from chromosome 6 variants from the phase 3 data of the 1000 Genomes Project [19]. This resulted in 5009 haplotype sequences of equal length (including the reference sequence) of approximately 171 million characters. We then discarded columns of identical characters, which reduced each sequence to approximately 5.38 million characters. We used an increasing number of these sequences as an input to our tool to verify its usability. The tests were run on a Ubuntu Linux 16.04 server. The server had 96 Intel Xeon E7-4830 v3 CPUs running at 2.10GHz and 1.4 TB of memory. Results on varying input sizes are shown in Fig. 3a. From this experiment it is conceivable that processing of thousands of complete human genomes takes only few CPU days. Figure 3b plots the number of founders against the number of segments. These look very promising, as using 130 founders instead of 5009 haplotypes as the input to pan-genome indexing of [22] will result into significant saving of resources; this solves the space bottleneck, and the preprocessing of founder reconstruction also saves time in the heavy indexing steps. The average segment length of some 1926 bases (171 million divided by 88778 segments) is also likely to be high enough not to break too badly the contiguity required for successful read alignment. To better see the contiguity of the resulting founder set, we mapped the haplotypes to the founders minimizing the number of jumps (simple greedy algorithm is optimal [15]). The result is shown in Fig. 3c. Since identical columns do not cause any jumps, we can now divide 171 million with 18274 jumps. This gives average distance between two jumps being 9358 bases. The heuristic part of optimizing the concatenation of founder blocks yields almost 5-fold improvement in the contiguity, compared to the worst case of each segment boundary yielding a discontinuity for each input sequence (which should be close to what a random concatenation order would produce).

Our intention was to compare our tool to an implementation of Ukkonen’s algorithm [15]. However, initial testing with four input sequences showed that the latter implementation is not practical with a data set of this size.

Our implementation is open source and available at the URL https://github.com/tnorri/founder-sequences.
The running time of our implementation plotted against the number of input sequences with $L = 10$. The data points have been fitted with a least-squares linear model, and the grey band shows the 95% confidence interval.

The founder and segment counts as produced by our implementation plotted against the number of input sequences with $L = 10$.

The average and median numbers of jumps, i.e. counts of positions where one needs to change from one founder sequence to another to read an original sequence, plotted against the number of input sequences with $L = 10$.

**Figure 3** Evaluation of founder reconstruction on a pan-genomic setting.

## 5 Discussion

With 5009 haplotypes reducing down to 130 founders with the average distance of two crossovers being 9358 bases, one can expect short read alignment and variant calling to become practical on such pan-genomic setting. We are investigating this on our tool *PanVC* [22], where one can simply replace its input multiple alignment with the one made of the founder sequences. With graph-based approaches, slightly more effort is required: Input variations are encoded with respect to the reference, so one first needs to convert variants into a multiple alignment, apply the founder reconstruction algorithm, and finally convert...
the multiple alignment of founder sequences into a directed acyclic graph. PanVC toolbox provides the required conversions. Alternatively, one can construct the pan-genome graph using other methods, and map the founder sequences afterwards to the paths of the graph: If original haplotype sequences are already spelled as paths, each founder sequence is a concatenation of existing subpaths, and can hence be mapped to a continuous path without alignment (possibly requiring adding a few missing edges).

Finally, it will be interesting to see how much the contiguity of the founder sequences can still be improved with different strategies for the concatenation order and with different formulations of the segmentation problem. For the former, we are investigating an approach with approximation guarantee. For the latter, we consider a variant with the number of founder sequenced fixed.

References

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A Proof of Lemma 4

Proof. Fix \( i \in [1, m] \). The \( i \)th iteration of the last loop in the algorithm computes the maximum in a range \( d_{k-1}[i', i] \), where \( d_{k-1}' \) is the original array \( d_{k-1} \) before modifications and \( i' = P[i] + 1 \) for some \( b \) and \( P \). Let \( \ell_i = i - i' \). Denote \( \tilde{\ell} = 1/m \sum_{i=1}^{m} \ell_i \), the “average query length.” We are to prove that the running time of the algorithm is \( O(m \log \tilde{\ell}) \), which implies the result since \( m \tilde{\ell} = \sum_{i=1}^{m} \ell_i \) and, obviously, \( \sum_{i=1}^{m} \ell_i \leq \sigma m \).

We say that a position \( j \) is touched if the function \( \text{maxd} \) is called with its first argument equal to \( j \). Clearly, it suffices to prove that the total number of touches is \( O(m \log \tilde{\ell}) \). While processing the query \( \text{maxd}(i-\ell_i, i) \), we may have touched many positions. Denote the sequence of all such position, for the given \( i \), by \( i_1, \ldots, i_r \); in other words, at the time of the query \( \text{maxd}(i-\ell_i, i) \), we have \( i_1 = i - \ell_i, i_j = a_{k-1}[i_{j-1}] \) for \( j \in [2, r] \), and \( i_r = i \). Obviously, \( i_1 < \cdots < i_r \). We say that, for \( j \in [1, r-1] \), the touch of \( i_j \) in the query \( \text{maxd}(i-\ell_i, i) \) is scaling if there exists an integer \( r \) such that \( i - i_j > 2^r \) and \( i - i_{j+1} \leq 2^r \) (see Figure 4). We count separately the total number of scaling and non-scaling touches in all \( i \).

![Figure 4 RMQ query on a range \([i - \ell_i, i]\); scaling touches are red.](image)

For position \( j \), denote by \( p(j) \) the number of non-scaling touches of \( j \). We are to prove that \( P = \sum_{j=1}^{m} p(j) \leq 2m \log \tilde{\ell} \). Let \( q_h(j) \) denote the value of \( a_{k-1}[j] - j \) in the \( h \)th non-scaling touch of \( j \), for \( h \in [1, p(j)] \). Suppose that this \( h \)th touch happens during the processing of a query \( \text{maxd}(i-\ell_i, i) \). By the definition, \( j + q_h(j) \) follows \( j \) in the sequence of touched positions. Since the touch of \( j \) is non-scaling, we have \( i - j > j + q_h(j) > 2^r \), where \( r \) is the largest integer such that \( i - j > 2^r \), and hence, \( q_h(j) < 2^r \). Since \( \text{maxd}(i-\ell_i, i) \) assigns \( a_{k-1}[j] \leftarrow i + 1 \), we have \( a_{k-1}[j] - j > i - j > 2^r \); after the query. In other words, we had \( a_{k-1}[j] - j = q_h(j) < 2^r \) before the query and have \( a_{k-1}[j] - j > 2^r \) after. This immediately implies that \( q_h(j) \geq 2^{h-1} \), for \( h \in [1, p(j)] \), and, therefore, every position can be touched in the non-scaling way at most \( O(\log m) \) times, implying \( P = O(m \log m) \). But we can deduce a stronger bound. Since the sum of all values \( j - a_{k-1}[j] \) for all positions \( j \) touched in a query \( \text{maxd}(i-\ell_i, i) \) is equal to \( \ell_i \), it is obvious that \( \sum_{j=1}^{m} p(j) \sum_{h=1}^{p(j)} q_h(j) \leq \sum_{i=1}^{m} \ell_i = m \tilde{\ell} \). On the other hand, we have \( \sum_{j=1}^{m} \sum_{h=1}^{p(j)} q_h(j) \geq \sum_{j=1}^{m} \sum_{h=1}^{2^r} q_h(j) = \sum_{j=1}^{m} 2^{p(j)} - m \). The well-known property of the convexity of the exponent is that the sum \( \sum_{j=1}^{m} 2^{p(j)} \) is minimized whenever all \( p(j) \) are equal and maximal, i.e., \( \sum_{j=1}^{m} 2^{p(j)} \geq \sum_{j=1}^{m} 2^{P/m} \). Hence, once \( P > 2m \log \tilde{\ell} \), we obtain \( \sum_{j=1}^{m} \sum_{h=1}^{p(j)} q_h(j) \geq \sum_{j=1}^{m} 2^{P/m} - m > m \tilde{\ell} - m \), which is larger than \( m \tilde{\ell} \) for \( \tilde{\ell} \geq 2 \) (the case \( \tilde{\ell} < 2 \) is trivial), contradicting \( \sum_{j=1}^{m} \sum_{h=1}^{p(j)} q_h(j) \leq m \tilde{\ell} \). Thus, \( P = \sum_{j=1}^{m} p(j) \leq 2m \log \tilde{\ell} \).

It remains to consider scaling touches. The definition implies that each query \( \text{maxd}(i-\ell_i, i) \) performs at most \( \log \ell_i \) scaling touches. Thus, it suffices to upperbound \( \sum_{i=1}^{m} \log \ell_i \). Since the function \( \log \) is concave, the sum \( \sum_{i=1}^{m} \log \ell_i \) is maximized whenever all \( \ell_i \) are equal and maximal, i.e., \( \sum_{i=1}^{m} \log \ell_i \leq \sum_{i=1}^{m} \log \left( \frac{1}{m} \sum_{j=1}^{m} \ell_j \right) = m \log \tilde{\ell} \), hence the result follows. ☐