Space-efficient merging of succinct de Bruijn graphs

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Abstract
We propose a new algorithm for merging succinct representations of de Bruijn graphs introduced in [Bowe et al. WABI 2012]. Our algorithm is inspired by the approach introduced by Holt and McMillan [Bionformatics 2014, ACM-BCB 2014] for merging Burrow-Wheeler transforms. In addition to its input, our algorithm uses only four bitvectors of working space and all data is accessed sequentially making the algorithm suitable for external memory execution. Our algorithm can also merge Colored succinct de Bruijn graphs, and can compute the Variable Order succinct representation from the plain representation of the input graphs.

Combining our merging algorithm with recent results on de Bruijn graph construction, we provide a space efficient procedure for building succinct representations of de Bruijn graphs for very large collections.

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1 Introduction

The de Bruijn graph for a collection of strings is a key data structure in genome assembly. After the seminal work of Bowe et al [5], many succinct representations of this data structure have been proposed in the literature [2][3][4][15] offering more and more functionalities still using a fraction of the space required to store the input collection uncompressed.

In this paper we consider the problem of merging two existing succinct representations of different collections in order to build the succinct de Bruijn graph for the union collection. Since from the de Bruijn graph is a lossy representation and it cannot be used to recover the

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original collection, the alternative to merging is storing a copy of the collection to be used for building new de Bruijn graphs.

Recently, Muggli et al. [14] have proposed a merging algorithm for colored de Bruijn graphs and have shown the effectiveness of the merging approach for the construction of de Bruijn graphs for very large datasets. The algorithm in [14] is based on a MSD Radix Sort procedure of the graph nodes and its running time is \( O(m \max(k, c)) \), where \( m \) is the total number of edges, \( k \) the order of the de Bruijn graph and \( c \) the total number of colors. In this paper we present a new merging algorithm based on LSD Radix Sort which is inspired by a BWT merging algorithm introduced by Holt and McMillan [9, 10] and later improved in [7]. Our algorithm has the same time complexity of the one in [14] but is space efficient, in that it only uses four bitvectors of working space, and accesses all data by sequential scans, so it is suitable for execution in external memory. In addition, our algorithm can compute, with no additional cost, the LCS (Longest Common Suffix) information thus making it possible to construct succinct Variable Order de Bruijn graph representations [4]. Combining our merging algorithm with recent results on external memory de Bruijn graph construction [6], we provide a space efficient procedure for building succinct representations of de Bruijn graphs for very large collections.

2 Notation

Given an alphabet \( \Sigma \) of size \( \sigma \) and a collection of strings \( S = s_1, \ldots, s_d \) over \( \Sigma \), we prepend to each string \( s_i \) \( k \) copies of a symbol \( \$ \notin \Sigma \) which is lexicographically smaller than any other symbol. The order-\( k \) de Bruijn graph \( G(V, E) \) for the collection \( S \) is a directed edge-labeled graph containing a node \( v \) for every unique \( k \)-mer appearing in one of the strings of \( S \). For each node \( v \) we denote by \( \overleftarrow{v} = v[1, k] \) its associated \( k \)-mer, where \( v[1] \ldots v[k] \) are symbols. The graph \( G \) contains an edge \((u, v)\), with label \( v[k] \), iff one of the strings in \( S \) contains a \((k + 1)\)-mer with prefix \( \overleftarrow{u} \) and suffix \( \overleftarrow{v} \). The edge \((u, v)\) therefore represents the \((k + 1)\)-mer \( u[1, k]v[k] \). Note that each node has at most \( |\Sigma| \) outgoing edges and all edges incoming to node \( v \) have label \( v[k] \).

2.1 BOSS succinct representation

In 2012, Bowe et al. [5] introduced a succinct representation for the de Bruijn graphs, herein referred to as BOSS representation, for the authors’ initials. The authors showed how to implement the graph in small space supporting fast navigation operations. The BOSS representation of the graph \( G(V, E) \) is defined by considering the set of nodes \( v_1, v_2, \ldots, v_n \) sorted according to the co-lexicographic order of the associated strings. Hence, if \( \overleftarrow{v} = v[k] \ldots v[1] \) denotes the string \( \overleftarrow{v} \) reversed, the nodes are ordered so that

\[
\overleftarrow{v}_1 < \overleftarrow{v}_2 < \cdots < \overleftarrow{v}_n
\]

By construction the first node is \( \overleftarrow{v}_1 = v_1[1, k] = \$^k \) and all \( \overleftarrow{v}_i \) are distinct. For each node \( v_i \), \( i = 1, \ldots, n \), we define \( W_i \) as the sorted sequence of symbols on the edges leaving from node \( v_i \); if \( v_i \) has out-degree zero we set \( W_i = \$ \). Finally, we define

1. \( W[1, m] \) as the concatenation \( W_1W_2\cdots W_n \);
2. \( W^-[1, m] \) as the bitvector such that \( W^-[i] = 1 \) iff \( W[i] \) corresponds to the label of the edge \((u, v)\) such that \( \overleftarrow{u} \) has the smallest rank among the nodes that have an edge going to node \( v \);
3. \( \text{last}[1, m] \) as the bitvector such that \( \text{last}[i] = 1 \) iff he outgoing edges in \( W[i] \) and \( W[i-1] \) have different source nodes, we define \( \text{last}[1] = 1 \).
It is easy to see that the length $m$ of the arrays $W$, $W^-$, and last is equal to the number of edges plus the number of nodes with out-degree 0. In addition, the number of 1's in last is equal to the number of nodes $n$, and the number of 1's in $W^-$ is equal to the number of nodes with positive in-degree, which is $n - 1$ since $v_1 = \$^S$ is the only node with in-degree 0. Note that there is a natural one-to-one correspondence $LF$ between the indices $i$ such that $W^-[i] = 1$ and the set $\{2, \ldots, n\}$: in this correspondence $LF(i) = j$ where $v_j$ is the destination node of the edge associated to the entry $W[i]$. See example in Figs. 1 and 2.

**Property 1.** The $LF$ map is order preserving in the following sense: if $W^-[i] = W^-[j] = 1$ then

\[
W[i] < W[j] \implies LF(i) < LF(j), \\
W[i] = W[j] \land (i < j) \implies LF(i) < LF(j).
\] (2)

In [5] it is shown that enriching the arrays $W$, $W^-$, and last with data structures supporting constant time rank and select operations [16, 8], we can efficiently navigate the graph $G$. The authors defined the following basic queries: $outgoing(v_i, c)$ returns the node $v_j$ reached from $v_i$ by an edge with label $c$, if no such node exists, it returns $-1$; $incoming(v_i)$ returns the nodes $v_j$ with an edge from $v_j$ with $v_i$; and $lastchar(v_i)$ returns the last symbol of $v_i$.

![Figure 1](image1.png)

**Figure 1** de Bruijn graph for $S = \{TACACT, TACTCA, GACTCA\}$

![Figure 2](image2.png)

**Figure 2** BOSS representation for $S = \{TACACT, TACTCA, GACTCA\}$
2.2 Colored BOSS

The colored de Bruijn graph \[11\] is an extension of the de Bruijn graphs for a multiset of individual graphs, where each edge is associated with a set of “colors” that indicates which graphs contain that edge.

The BOSS representation for a set of graphs \[G = \{G_1, \ldots, G_t\}\] contains the union of all individual graphs. The colors of each edge \(W[i]\) are stored in a two-dimensional binary array \(C\), such that \(C[i,j] = 1\) indicates that the \(i\)-th edge is present in the individual de Bruijn graph \(G_j\). There are different compression alternatives for the color matrix \(C\) that support fast operations \[13, 2, 13\]. Recently, Alipanah et al. \[1\] presented a different approach to reduce the size of \(C\) by recoloring.

2.3 Variable-order BOSS

The order \(k\) (dimension) of a de Bruijn graph is an important parameter for genome assembling algorithms. The graph can be very small and uninformative when \(k\) is small, whereas it can become too large with unrelated parts when \(k\) is large.

To add flexibility to the BOSS representation, Boucher et al. \[4\] suggest to enrich the BOSS representation of an order-\(k\) de Bruijn graph with the length of the longest common suffix (LCS) between the consecutive nodes \(v_1, v_2, \ldots, v_n\) sorted according to Eq. 1. These lengths are stored in a wavelet tree using \(O(n \log k)\) additional bits. The authors show that this enriched representation supports navigation on all de Bruijn graphs of order \(k' \leq k\) and that it is even possible to vary the order \(k'\) of the graph on the fly during the navigation up to the maximum value \(k\).

The LCS between \(\overleftarrow{v_i}\) and \(\overleftarrow{v_{i+1}}\) is equivalent to the length of the longest common prefix (LCP) between their reverses \(\overrightarrow{v_i}\) and \(\overrightarrow{v_{i+1}}\). The LCP (or LCS) between the nodes \(v_1, v_2, \ldots, v_n\) can be computed during the \(k\)-mer sorting phase. In the following we denote by VO-BOSS the variable order succinct de Bruijn graph consisting of the BOSS representations enriched with the LCS/LCP information.

3 Merging plain BOSS representations

Suppose we are given the BOSS representation of two de Bruijn graphs \(\langle W_0, W_0^-, \text{last}_0 \rangle\) and \(\langle W_1, W_1^-, \text{last}_1 \rangle\) obtained respectively from the collections of strings \(C_0\) and \(C_1\). In this section we show how to compute the BOSS representation for the union collection \(C_{01} = C_0 \cup C_1\). The procedure does not change in the general case when we are merging an arbitrary number of graphs. Let \(G_0\) and \(G_1\) denote respectively the (uncompressed) de Bruijn graphs for \(C_0\) and \(C_1\), and let

\[v_1, \ldots, v_{n_0}\] and \[w_1, \ldots, w_{n_1}\]

their respective set of nodes sorted in colexicographic order. Hence, with the notation of the previous section we have

\[\overleftarrow{v_1} < \cdots < \overleftarrow{v_{n_0}}\] and \[\overleftarrow{w_1} < \cdots < \overleftarrow{w_{n_1}}\] (3)

We observe that the \(k\)-mers in the collection \(C_{01}\) are simply the union of the \(k\)-mers in \(C_0\) and \(C_1\). To build the de Bruijn graph for \(C_{01}\) we need therefore to: 1) merge the nodes in \(G_0\) and \(G_1\) according to the colexicographic order of their associated \(k\)-mers, 2) recognize when two nodes in \(G_0\) and \(G_1\) refer to the same \(k\)-mer, and 3) properly merge and update the bitvectors \(W_0^-, \text{last}_0\) and \(W_1^-, \text{last}_1\). The following sections are devoted to the solutions of each one of these subproblems.
3.1 Phase 1: Merging \( k \)-mers

The main technical difficulty is that in the BOSS representation the \( k \)-mers associated to each node \( x = v[1,k] \) are not directly available. Our algorithm will essentially reconstruct them using the symbols associated to the graph edges; note that to this end it suffices to consider the edges such that the corresponding entry in \( W_0^c \) or \( W_1^c \) is equal to 1.

Following these edges, first we can recover the last symbol of each \( k \)-mer, following them a second time we could recover the last two symbols of each \( k \)-mer and so on. However, to save space we do not explicitly maintain the \( k \)-mers; instead, using the ideas from \( \cite{9} \) \( \cite{10} \) we compute a bitvector \( Z^{(c)} \) representing how the \( k \)-mers in \( G_0 \) and \( G_1 \) should be merged according to the colexicographic order. In addition, we maintain just enough information, to recognize when two \( k \)-mers are identical, so that their incoming and outgoing edges can be merged.

To this end, our algorithm executes \( k - 1 \) iterations of the code shown in Fig. 3. For \( h = 2, 3, \ldots, k \), during iteration \( h \), we compute a bitvector \( Z^{(h)}[1,n_0 + n_1] \) containing \( n_0 \) 0’s and \( n_1 \) 1’s such that \( Z^{(h)} \) satisfies the following property

**Property 2.** For \( i = 1, \ldots, n_0 \) and \( j = 1, \ldots, n_1 \) the \( i \)-th 0 precedes the \( j \)-th 1 in \( Z^{(h)} \) if and only if \( W^{c}[1,h] \preceq W^{c}[1,h] \).

Property 2 states that if we merge the nodes from \( G_0 \) and \( G_1 \) according to the bitvector \( Z^{(h)} \), the corresponding \( k \)-mers will be sorted according to the colexicographic order restricted to the first \( h \) symbols of each reversed \( k \)-mer. As a consequence, \( Z^{(k)} \) will provide us the colexicographic order of all the nodes in \( G_0 \) and \( G_1 \). To prove that Property 2 holds, we first define \( Z^{(1)} \) and show that it satisfies the property, then we prove that for \( h = 2, \ldots, k \) the code in Fig. 3 computes \( Z^{(k)} \) that still satisfies Property 2.

For \( c \in \Sigma \) let \( \ell_0(c) \) and \( \ell_1(c) \) denote respectively the number of nodes in \( G_0 \) and \( G_1 \) whose associated \( k \)-mers end with symbol \( c \). These values can be computed with a single scan of \( W_0 \) (resp. \( W_1 \)) considering only the symbols \( W_0[i] \) (resp. \( W_1[i] \)) such that \( W_0^{-1}[i] = 1 \) (resp. \( W_1^{-1}[i] = 1 \)). By construction, it is

\[
n_0 = 1 + \sum_{c \in \Sigma} \ell_0(c), \quad n_1 = 1 + \sum_{c \in \Sigma} \ell_1(c)
\]

where the two 1’s account for the nodes \( v_1 \) and \( w_1 \) whose associated \( k \)-mer is \( \$^{k} \). We define

\[
Z^{(1)} = 01^{\ell_0(1)}1^{\ell_1(1)}0^{\ell_0(2)}1^{\ell_1(2)}\ldots 0^{\ell_0(\sigma)}1^{\ell_1(\sigma)}
\]

the first pair \( 01 \) in \( Z^{(1)} \) accounts for \( v_1 \) and \( w_1 \); each group \( 0^{\ell_0(c)}1^{\ell_1(c)} \) accounts for the nodes ending with symbol \( c \). Note that, apart from the first two symbols, \( Z^{(1)} \) can be logically partitioned into \( \sigma \) subarrays one for each alphabet symbol. For \( c \in \Sigma \) let

\[
\text{start}(c) = 3 + \sum_{i < c} (\ell_0(i) + \ell_1(i))
\]

then the subarray corresponding to \( c \) starts at position \( \text{start}(c) \) and has size \( \ell_0(c) + \ell_1(c) \). Note that, as a consequence of \( \cite{3} \), the \( i \)-th 0 (resp. \( j \)-th 1) belongs to the subarray associated to symbol \( c \) if \( W^{c}[1] = c \) (resp. \( W^{c}[1] = c \)).

To see that \( Z^{(1)} \) satisfies Property 2 observe that the \( i \)-th 0 precedes \( j \)-th 1 iff the \( i \)-th 0 belongs to a subarray corresponding to a symbol not larger than the symbol corresponding to the subarray containing the \( j \)-th 1; this implies \( W^{c}[1,1] \succeq W^{c}[1,1] \).

The bitvectors \( Z^{(h)} \) computed by the algorithm in Fig. 3 can be logically divided into the same subarrays we defined for \( Z^{(1)} \). Because of how the array \( F \) is initialized and updated,
we see that every time we read a symbol \( c \) at line 14 the corresponding bit \( b = Z^{(h-1)}[k] \), identifying the graph containing \( c \), is written in the portion of \( Z^{(h)} \) corresponding to \( c \) (line 16). The only exception are the first two entries of \( Z^{(h)} \) which are written at line 6 which corresponds to the nodes \( v_1 \) and \( w_1 \). We treat these nodes differently since they are the only ones with in-degree zero. For all other nodes, we implicitly use the one-to-one correspondence between entries \( W[i] \) with \( W^−[i] = 1 \) and nodes \( v_j \) with positive in-degree.

Note that lines 8–10 and 17–22 of the algorithm are related to the computation of the \( B \) array which is used in the following section and do not influences the computation of \( Z^{(h)} \) or Property 2. We can now formally prove the following result.

\[\text{Lemma 3. For } h = 2, \ldots, k, \text{ the array } Z^{(h)} \text{ computed by the algorithm in Fig. 3 satisfies Property 2.} \]

**Proof.** To prove the “if” part, let \( 1 \leq f < g \leq n_0 + n_1 \) denote two indexes such that \( Z^{(h)}[f] \) is the \( i \)-th 0 and \( Z^{(h)}[g] \) is the \( j \)-th 1 in \( Z^{(h)} \) for some \( 1 \leq i \leq n_0 \) and \( 1 \leq j \leq n_1 \). We need to show that \( \overrightarrow{v_i}[1, h] \leq \overrightarrow{w_j}[1, h] \).

Assume first \( \overrightarrow{v_i}[1] \neq \overrightarrow{w_j}[1] \). The hypothesis \( f < g \) implies \( \overrightarrow{v_i}[1] < \overrightarrow{w_j}[1] \), since otherwise during iteration \( h \) the \( j \)-th 1 would have been written in a subarray of \( Z^{(h)} \) preceding the one where the \( i \)-th 0 is written. Hence \( \overrightarrow{v_i}[1, h] \leq \overrightarrow{w_j}[1, h] \) as claimed.

Assume now \( \overrightarrow{v_i}[1] = \overrightarrow{w_j}[1] = c \). In this case during iteration \( h \) the \( i \)-th 0 and the \( j \)-th 1 are both written to the subarray of \( Z^{(h)} \) associated to symbol \( c \). Let \( f', g' \) denote respectively the value of the main loop variable \( p \) in the procedure of Fig. 3 when the entries \( Z^{(h)}[f] \) and \( Z^{(h)}[g] \) are written. Since each subarray in \( Z^{(h)} \) is filled sequentially, the hypothesis \( f < g \) implies \( f' < g' \). By construction \( Z^{(h-1)}[f'] = 0 \) and \( Z^{(h-1)}[g'] = 1 \). Say \( f' \) is the \( i' \)-th 0 in \( Z^{(h-1)} \) and \( g' \) is the \( j' \)-th 1 in \( Z^{(h-1)} \). By the inductive hypothesis on \( Z^{(h-1)} \) it is

\[\overrightarrow{v_i}[1, h - 1] \leq \overrightarrow{w_j}[1, h - 1]. \tag{4}\]

By construction there is an edge labeled \( c \) from \( v_{i'} \) to \( v_i \) and from \( w_{j'} \) to \( w_j \) hence

\[\overrightarrow{v_i}[1, h] = \overrightarrow{v_i'}[1, h - 1]c, \quad \overrightarrow{w_j}[1, h] = \overrightarrow{w_j'}[1, h - 1]c; \]

therefore

\[\overrightarrow{v_i}[1, h] = c\overrightarrow{v_i'}[1, h - 1], \quad \overrightarrow{w_j}[1, h] = c\overrightarrow{w_j'}[1, h - 1]; \]

using (4) we conclude that \( \overrightarrow{v_i}[1, h] \leq \overrightarrow{w_j}[1, h] \) as claimed.

For the “only if” part assume \( \overrightarrow{v_i}[1, h] \leq \overrightarrow{w_j}[1, h] \) for some \( i \geq 1 \) and \( j \geq 1 \). We need to prove that in \( Z^{(h)} \) the \( i \)-th 0 precedes the \( j \)-th 1. If \( \overrightarrow{v_i}[1] \neq \overrightarrow{w_j}[1] \) the proof is immediate. If \( c = \overrightarrow{v_i}[1] = \overrightarrow{w_j}[1] \) then

\[\overrightarrow{v_i}[2, h] \leq \overrightarrow{w_j}[2, h]. \]

Let \( i' \) and \( j' \) be such that \( \overrightarrow{v_i'}[1, h - 1] = \overrightarrow{v_i}[2, h] \) and \( \overrightarrow{w_j'}[1, h - 1] = \overrightarrow{w_j}[2, h] \). By induction hypothesis, in \( Z^{(h-1)} \) the \( i' \)-th 0 precedes the \( j' \)-th 1.

During phase \( h \), the \( i \)-th 0 in \( Z^{(h)} \) is written to position \( f \) when processing the \( i' \)-th 0 of \( Z^{(h-1)} \), and the \( j \)-th 1 in \( Z^{(h)} \) is written to position \( g \) when processing the \( j' \)-th 1 of \( Z^{(h-1)} \). Since in \( Z^{(h-1)} \) the \( i' \)-th 0 precedes the \( j' \)-th 1 and since \( f \) and \( g \) both belong to the subarray of \( Z^{(h)} \) corresponding to the symbol \( c \), their relative order does not change and the \( i \)-th 0 precedes the \( j \)-th 1 as claimed.
3.2 Phase 2: Recognizing identical $k$-mers

Once we have determined, via the bitvector $Z^{(h)}[1, n_0 + n_1]$, the colexicographic order of the $k$-mers, we need to determine when two $k$-mers are identical since in this case we have to merge their outgoing and incoming edges. Note that two identical $k$-mers will be consecutive in the colexicographic order and they will necessarily belong one to $G_0$ and the other to $G_1$.

Following Property 2 and a technique introduced in [7], we identify the $i$-th $0$ in $Z^{(h)}$ with $W_{j}$ and the $j$-th $1$ in $Z^{(h)}$ with $W_{j}$. Property 2 is equivalent to state that we can logically partition $Z^{(h)}$ into $b(h) + 1$ $h$-blocks

$$Z^{(h)}[1, \ell_1], Z^{(h)}[\ell_1 + 1, \ell_2], \ldots, Z^{(h)}[\ell_{b(h)} + 1, n_0 + n_1]$$

such that each block corresponds to a set of $k$-mers which are prefixed by the same length-$h$ substring. Note that during iterations $h = 2, 3, \ldots, k$ the $k$-mers within an $h$-block will be rearranged, and sorted according to longer and longer prefixes, but they will stay within the same block.

In the algorithm of Fig. 3, in addition to $Z^{(h)}$, our algorithm maintains an integer array $B[1, n_0 + n_1]$, such that at the end of iteration $h$ it is $B[i] \neq 0$ if and only if a block of $Z^{(h)}$ starts at position $i$. At the beginning of the algorithm we set $B = 101010 \ldots 10^{b(h)+1}10^{b(h)+1}$. During iteration $h$ new block boundaries are established as follows. At line 8 identify each existing block with its starting position. Then, at lines 17-22 if the entry $Z^{(h)}[q]$ has the form $c\alpha$, while $Z^{(h)}[q - 1]$ has the form $c\beta$ with $\alpha$ and $\beta$ belonging to different blocks, then
we know that \( q \) is the starting position of an \( h \)-block. Note that we write \( h \) to \( B[q] \) only if no other value has been previously written there. This ensures that \( B[q] \) is the smallest position in which the string in \( Z^{(h)}[q-1] \) and \( Z^{(h)}[q] \) differ, or equivalently, \( B[q] = h - 1 \) is the LCP between the strings in \( Z^{(h)}[q-1] \) and \( Z^{(h)}[q] \). The above observations are summarized in the following Lemma, which is a generalization to de Bruijn graphs of an analogous result for BWT merging established in Corollary 4 in [7].

\[ \text{Lemma 4.} \quad \text{After iteration } h \text{ of our merging algorithm for } q = 2, \ldots, n_0 + n_1 \text{ if } B[q] \neq 0 \text{ then } B[q] - 1 \text{ is the LCP between the reverse } k \text{-mers associated to } Z^{(h)}[q-1] \text{ and } Z^{(h)}[q] \text{".} \]

The above lemma shows that using array \( B \) we can establish when two \( k \)-mers are equal and consequently the associated graph nodes should be merged.

### 3.3 Phase 3: Building the succinct representation for the union graph

We now show how to compute the succinct representation of the union graph \( G_0 \cup G_1 \), consisting of the arrays \((W_{01}, W_{01}^{-}, \text{last}_{01})\), given the succinct representations of \( G_0 \) and \( G_1 \) and the arrays \( Z^{(h)} \) and \( B \).

The arrays \( W_{01}, W_{01}^{-}, \text{last}_{01} \) are initially empty and we will fill them in a single sequential pass. For \( q = 1, \ldots, n_0 + n_1 \) we consider the values \( Z^{(h)}[q] \) and \( B[q] \). If \( B[q] = 0 \) then the \( k \)-mer associated to \( Z^{(h)}[q-1] \), say \( v_i \), is identical to the \( k \)-mer associated to \( Z^{(h)}[q] \), say \( v_j \). In this case we recover from \( W_0 \) and \( W_1 \) the labels of the edges outgoing from \( v_i \) and \( v_j \), we compute their union and write them to \( W_{01} \) (we assume the edges are in the lexicographic order), writing at the same time the representation of the resulting out-degree of the new node to \( \text{last}_{01} \). If instead \( B[q] \neq 0 \), then the \( k \)-mer associated to \( Z^{(h)}[q-1] \) is unique and we copy the information of its outgoing edges and out-degree directly to \( W_{01} \) and \( \text{last}_{01} \).

When we write the symbol \( W_{01}[i] \) we simultaneously write the bit \( W_{01}^{-}[i] \) according to the following strategy. If the symbol \( c = W_{01}[i] \) is the first occurrence of \( c \) after a value \( B[q] \), with \( 0 < B[q] < k \), then we set \( W_{01}^{-}[i] = 1 \), otherwise we set \( W_{01}^{-}[i] = 0 \). The rationale is that if no values \( B[q] \) with \( 0 < B[q] < k \) occur between two nodes, then the associated (reversed) \( k \)-mers have a common LCP of length \( k - 1 \) and therefore if they both have an outgoing edge labelled with \( c \) they reach the same node and only the first one should have \( W_{01}^{-}[i] = 1 \).

### 4 Implementation details and analysis

Let \( n = n_1 + n_0 \) denote the sum of number of nodes in \( G_0 \) and \( G_1 \), and let \( m = |W_0| + |W_1| \) denote the sum of the number of edges. The \( k \)-mer merging algorithm as described executes in \( \mathcal{O}(m) \) time a first pass over the arrays \( W_0, W_0^{-}, \) and \( W_1, W_1^{-} \) to compute the values \( \ell_0(c) + \ell_1(c) \) for \( c \in \Sigma \) and initialize the arrays \( \text{start}[1, \sigma] \) and \( Z^{(1)}[1, n] \) (Phase 1). Then, the algorithm executes \( k - 1 \) iterations of the code in Fig. 3 each iteration taking \( \mathcal{O}(m) \) time. Finally, still in \( \mathcal{O}(m) \) time the algorithm computes the succinct representation of the union graph (Phases 2 and 3). The overall running time is therefore \( \mathcal{O}(mk) \).

The space usage of the algorithm, in addition to the input and the output consists of \( 2n \) bits for two instances of the \( Z^{(1)} \) array (for the current \( Z^{(h)} \) and for the previous iteration \( Z^{(h-1)} \)), plus \( \mathcal{O}(n \log k) \) bits for the \( B \) array. Note however, that during iteration \( h \) we only need to check whether \( B[i] \) is equal to 0, \( h \), or some value within 0 and \( h \). Similarly, for the computation of \( W_{01}^{-} \) we need to distinguish between the cases where \( B[i] \) is equal to 0, \( k \) or some value \( 0 < B[i] < k \). Therefore, we can save space replacing \( B[1, n] \) with an array \( B_2[1, n] \) containing two bits per entry representing the four possible states \( \{0, 1, 2, 3\} \). During
iteration $h$, the values in $B_2$ are used instead of the ones in $B$ as follows: An entry $B_2[i] = 0$ corresponds to $B[i] = 0$, an entry $B_2[i] = 3$ corresponds to an entry $0 < B[i] < h - 1$. In addition, if $h$ is even, an entry $B_2[i] = 2$ corresponds to $B[i] = h$ and an entry $B_2[i] = 1$ corresponds to $B[i] = h - 1$; while if $h$ is odd the correspondence is $2 \to h - 1, 1 \to h$. The reason for this apparently involved scheme, first introduced in [6], is that during phase $h$, an entry in $B_2$ can be modified either before or after we have read it at Line 8. Using this technique, we get that the total working space of the algorithm, i.e., the space in addition to the input and the output is $4n + O(1)$ bits.

Note that during Phase 1, at each iteration $h = 2, \ldots, k$, the arrays $(W_0, W_0^-, last_0)$, $(W_1, W_1^-, last_1)$, $Z^{(h-1)}$, and $B_2$ are read sequentially from beginning to end. At the same time, the arrays $Z^{(h)}[1, n]$ and $B_2$ are written sequentially but into $\sigma$ different partitions whose starting positions are the values in start and are the same for each iteration. Thus, if we split $Z^{(h)}$ and $B_2$ into $\sigma$ different files all accesses are sequential and Phase 1 is suitable for execution in external memory using only $O(\sigma)$ words of RAM for the arrays start, $F$, and Block_id. Since during Phases 2 and 3 all input and output arrays are accessed sequentially in linear time we can summarize our analysis as follows.

$\blacktriangleright$ \textbf{Theorem 5.} The merging of two succinct representations of de Bruijn graphs takes $O(nk)$ time and $4n + O(\sigma \log m)$ bits of working space. The algorithm can be executed in external memory using $O(\sigma \log m)$ bits of RAM and $O(mk)$ sequential I/Os. $\blacktriangleleft$

Note that the $k$-mer merging algorithm uses only symbols in $(W_0, last_0)$ and $(W_1, last_1)$ corresponding to the $1$‘s in $W_0^-$ and $W_1^-$ (line 13 in Fig. 3). Before starting Phase 1 we can make a copy of such arrays in temporary arrays $(W_0[1, n_0], last_0[1, n_0])$ and $(W_1[1, n_1], last_1[1, n_1])$, so that each successive iteration takes $O(n)$ time. The overall running time can be therefore reduced to $O(m + nk)$, at the cost of using $2n(1 + \lceil \log \sigma \rceil)$ additional bits.

$\blacktriangleright$ \textbf{Theorem 6.} The merging of two succinct representations of de Bruijn graphs can be done in $O(m + nk)$ time and $2n(1 + \lceil \log \sigma \rceil) + O(\sigma \log m)$ bits of working space. The algorithm can be executed in external memory using $O(\sigma \log m)$ bits of RAM and $O(m + nk)$ sequential I/Os. $\blacktriangleleft$

5 \hspace{1cm} \textbf{Merging other BOSS representations}

Our algorithm can be easily generalized to merge colored/variable-order BOSS representations, described in Sections 4.2 and 4.3.

Given the colored BOSS representation of two de Bruijn graphs $G_0$ and $G_1$, the corresponding color matrices $C_0$ and $C_1$ have size $m_0 \times c_0$ and $m_1 \times c_1$, respectively. We initially create a new color matrix $C_{01}$ of size $(m_1 + m_2) \times (c_0 + c_1)$ with all entries empty. During the merging of the union graph (Phase 3), for $q = 1, \ldots, n$, we write the colors of the edges associated to $Z^{(h)}[q]$ to the corresponding line in $C_{01}$ possibly merging the colors when we find nodes with identical $k$-mers in $O(c_{01})$ time, with $c_{01} = c_0 + c_1$. To make sure that colors from $C_0$ and $C_1$ do not intersect in the new graph we just need to add the constant $c_0$ (the number of distinct colors in $G_0$) to any color id coming from the matrix $C_1$.

$\blacktriangleright$ \textbf{Theorem 7.} The merging of two succinct representations of colored de Bruijn graphs takes $O(m \cdot \max(k, c_{01}))$ time and $4n + O(\sigma \log m)$ bits of working space, where $c_{01}$ is $c_0 + c_1$. $\blacktriangleleft$

We now show that we can compute the variable order VO-BOSS representation of the union of two de Bruijn graphs $G_0$ and $G_1$ given their plain, e.g. non variable order, BOSS representations. For the VO-BOSS representation we need the LCS array for the nodes in the
union graph \((W_{01}, W_{01}^{-}, \text{last}_{01})\). We notice that after merging the \(k\)-mers of \(G_0\) and \(G_1\) with the algorithm in Fig. 3 (Phase 1) the values in \(B[1,n]\) already provide the LCP information between the reverse labels of all consecutive nodes (Lemma 4). When building the union graph during Phase 3, for \(q = 1, \ldots, n\), the LCS between two consecutive nodes, say \(v_i\) and \(w_j\), is equal to the LCP of their reverses \(\overrightarrow{v_i}\) and \(\overrightarrow{w_j}\), which is given by \(B[q - 1]\) whenever \(B[q] > 0\) (if \(B[q] = 0\) then \(\overrightarrow{v_i} = \overrightarrow{w_j}\) and nodes \(v_i\) and \(v_j\) should be merged). Note that in this case we cannot use the compact (2-bit) representation of \(B\) suggested in Section 4, however we can re-use the space of \(B[1,n]\) to store the LCS array.

\textbf{Theorem 8.} The merging of two succinct representations of variable order de Bruijn graphs takes \(O(mk)\) time and \(2n + O(\sigma \log m)\) bits of working space.

\section{Space-efficient construction of succinct de Bruijn graphs}

Using our merging algorithm it is straightforward to design a complete space-efficient algorithm to construct succinct de Bruijn graphs.

Assume we are given a string collection \(S = s_1, \ldots, s_d\) of total length \(N\), and the desired order \(k\), and the amount of available RAM \(M\). First, we split \(S\) into smaller subcollections \(r_1 = s_{j_1}, \ldots, s_{j_1}'\), such that we can compute the BWT and LCP array of each subcollection in linear time in RAM using \(M\) bytes, using \(e.g.\) the suffix sorting algorithm \(gSACA-K\) \cite{12}. For each subcollection we then compute, and write to disk, the BOSS representation of its de Bruijn graph using the algorithm described in \cite[Section 5.3]{3}. Since these are linear algorithms the overall cost of this phase is \(O(N)\) time and \(O(N)\) sequential IOs.

Finally, we merge all de Bruijn graphs into a single BOSS representation of the union graph with the external memory variant of the merging algorithm (Section 3). Since the number of subcollections is \(O(N/M)\), a total of \(\log(N/M)\) merging rounds will suffices to get the BOSS representation of the union graph.

\textbf{Theorem 9.} Given a collection of strings collection \(S = s_1, \ldots, s_d\) of total length \(N\), the construction of the succinct order \(k\) de Bruijn graph takes \(O(Nk \log(N/M))\) time using \(O(M)\) words of RAM.

Note that our construction algorithm can be extended to generate colored/variable order variants of the de Bruijn graph, since the last merging step can compute these variants given plain BOSS representations as input (see Section 5). Finally, we observe that we can also update the de Bruijn graph built for a collection \(S\) with new data without reconstructing the complete graph. In order to do that, we can compute the succinct de Bruijn graph for the new strings (via the BWT and LCP array) and then merge the new graph into the larger de Bruijn graph for \(S\) using the merging algorithm.

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