Burrows-Wheeler transformations and de Bruijn words

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Abstract

We formulate and explain the extended Burrows-Wheeler transform of Mantaci et al from the viewpoint of permutations on a chain taken as a union of partial order-preserving mappings. In so doing we establish a link with syntactic semigroups of languages that are themselves cyclic semigroups. We apply the extended transform with a view to generating de Bruijn words through inverting the transform. We also make use of de Bruijn words to facilitate a proof that the maximum number of distinct factors of a word of length $n$ has the form $\frac{1}{2}n^2 - O(n \log n)$.

1 Introduction

1.1 Definitions and Example

The original notion of a Burrows-Wheeler (BW) transform, introduced in [2], has become a major tool in lossless data compression. It replaces a primitive word $w$ (one that is not a power of some other word) by another word $BW(w)$ of the same length over the same alphabet but in a way that is generally rich in letter repetition and so lends to easy compression. Moreover the transform can be inverted in linear time; see for example [3]. Unfortunately, not all words arise as Burrows-Wheeler transforms of a primitive word so, in the original format, it was not possible to invert an arbitrary string. The extended BW transform however does allow the inversion of an arbitrary word and the result in general is a multiset (a set allowing repeats)
of necklaces, which are conjugacy classes of primitive words. This was first explicitly introduced in [8] by Mantaci et al. based on the bijection between these two collections first enunciated by Gessel and Reutenauer in [5].

In this opening section we will explain and prove the existence of the extended transform in a fashion that emphasises the approach whereby a permutation on a finite chain is expressed as a disjoint union of one-to-one partial order-preserving mappings.

**Notation and Background** The underlying base set for our mappings will be the finite chain $[n] = \{0 < 1 < \cdots < n-1\}$. As usual $A^*$ will stand for the free monoid over $A = \{a_0, a_1, \cdots\}$, which is simply the set of all words, or strings, over the alphabet $A$ together with the empty word $\varepsilon$, although throughout this paper we assume a fixed order $a_0 < a_1 < \cdots$ for $A$. The free semigroup is denoted by $A^+ = A^* \setminus \{\varepsilon\}$. For emphasis, we sometimes denote equality of $u, v \in A^+$ by $u \equiv v$. The set of letters that occur at least once in $w \in A^*$ is known as the content of $w$, denoted by $c(w)$. Following [8] we shall denote the first and last letters of a word $w \in A^+$ respectively by $F(w)$ and $L(w)$. In general, the $i$th letter of a word $w$ is written as $(w)_i$. The number of instances of the letter $a_i$ in a word $w$ will be denoted by $|w|_{a_i}$, while the length of $w$ is written $|w|$. We say that $w$ is primitive if $w$ is not a power of some other word. A word $u \in A^+$ is a factor of $w \in A^+$ if $w \in A^* u A^*$; $u$ is an $m$-factor of $w$ if additionally $u \in A^m$. We call $u$ a prefix (respectively suffix) of $w$ if $w \in u A^*$ (respectively $w \in A^* u$). A subword of $w$ is any word that may be formed by deletion of some of the letters of $w$; it follows that the factors of $w$ represent a special class of subwords of $w$.

A standard text for results concerning combinatorics on words is [7] in which may be found proofs for simple unproved assertions concerning roots and conjugates that follow. If $w = wv, (u, v \in A^*)$ we say that $w' = vu$ is a conjugate of $w$. The relation $\sim$ on $A^*$ whereby $w \sim w'$ if $w'$ is a conjugate of $w$ is an equivalence relation on $A^*$. In the case of a primitive word $w$, the equivalence classes of $\sim$ are known as necklaces, and we denote the necklace of a word $w$ by $n(w)$; the length of $n(w)$ is $|w|$, which is also the cardinal of the necklace as $w$ is primitive. The first word of $n(w)$ in the lexicographic order is known as its Lyndon word. A border of a word $w$ is word $u \in A^+$ such that $w \in u A^+ \cap A^+ u$. No Lyndon word has a border (see Proposition 2.2(iii)).
The root of a word \( w \) is the shortest factor \( r = \text{root}(w) \) of \( w \) such that \( w = r^t \) for some \( t \geq 1 \). Two words \( w \) and \( u \) commute in \( A^+ \) if and only if they share a common root, which is in turn equivalent to the condition that \( w \) and \( u \) have a common power. The number of distinct conjugates of a word \( w \) equals the length of \( \text{root}(w) \) and \( \text{root}(w') \), the root of a conjugate \( w' \) of \( w \), is a conjugate of \( \text{root}(w) \).

For a word \( w \) we denote the infinite one-sided word \( wwww \cdots \) by \( w^\omega \) with the notion of factor extending in the obvious way. Note that \( u^\omega = v^\omega \) if and only if \( \text{root}(u) = \text{root}(v) \). The factors \( u \) of \( w^\omega \) of finite length are the power factors of \( w \); a power factor for which \( |u| \leq |w| \) is a cyclic factor of \( w \): equivalently \( u \) is a factor of some conjugate of \( w \).

The interval \( I = [i, j] \) of a chain \( X \) is the subset \( I = \{ k : i \leq k \leq j \} \). A mapping \( \alpha \), the domain and range of which are both subsets of \( A \), is order-preserving if when \( a \cdot \alpha \) and \( b \cdot \alpha \) are both defined, \( \alpha \) satisfies the condition:

\[
a \leq b \rightarrow a \cdot \alpha \leq b \cdot \alpha \ (a, b \in A).
\]

We shall frequently use the action notation, \( a \cdot \alpha \) as opposed to juxtaposition \( aa \alpha \) when the symbol on the right is a function and not a product in \( A^* \) (although a central dot is also used at times simply as a visual separator within a word). Mapping composition is written from left to right. Here we write \( PI_n \) to denote the (inverse) semigroup of all partial one-to-one mappings on \([u]\), and we denote the (inverse) subsemigroup of all order-preserving members of \( PI_n \) by \( POI_n \).

**Example 1.1** We give an example, following [8], that illustrates how to effect the bijection from multisets of necklaces to words and how to reverse this process. Let our alphabet be \( A = \{ a < b \} \) and let the set of Lyndon words of our necklaces be \( M = \{ aab, ab, abb \} \). Consider the collection of all words of the form \( u^\omega w \), where \( u \in n(v) \) \( (v \in M) \) and \( l \) is the least common multiple of the lengths of the words of \( M \): in this instance \( l = 3 \times 2 = 6 \). All these words then have common length \( l \). We order this set of words lexicographically to yield, in our example, the following array.
The Burrows-Wheeler transform of $M$ is then the word formed by the $l$th column of the table, read from the top, which in this case gives $BW(M) = babbaaba$. The word $BW(M)$ is also formed by the list of last letters $L(u)$: both renditions of $BW(M)$ are highlighted in bold in the table. In [8] $BW(M)$ was defined by the letters $L(u)$. Their definition was also framed in context of the infinite table $T$ of rows $u^\omega$, which simply consists of the table of the first $l$ columns of $T$, as defined above, repeated infinitely often. However, as explained in [8], the table does not need to be extended to $l$ columns in order to determine the order of the rows: by a theorem of Wilf and Fine on word periodicity, the order of two rows that are respective powers of the root words $u$ and $v$ matches the lexicographic order of their prefixes of length $k = |u| + |v| - \gcd(|u|, |v|)$ (and this bound is tight). Hence the number of columns required in order to determine the row order of the table is always less than the sum of the lengths of the longest two necklaces of the multiset.

The formal use of the lcm $l$ here allows us to define $BW(M)$ as a specified column of the table, which is a conceptual convenience used in our proofs. The stipulation that the words of $M$ be primitive is necessary in order that the $BW$ transform be one-to-one. Note that the roots of the words are not in lexicographic order: the root $baa$ precedes the root $ba$ in the table. However, the Lyndon roots do appear in lexicographic order: $aab < ab < abb$ both lexicographically and in the rows of the table (see Theorem 1.2.13).

We recover the set $M$ from $w = BW(M)$ by way of the so-called standard permutation $\pi = \pi(w)$. To construct $\pi$, take the first column of the table, which consists of the content of the words of $M$ arranged in alphabetical order with the number of occurrences of a letter equal to the number of instances of that letter among the Lyndon words of $M$. In our example the column of first letters forms the word $F(M) = aaaaabbbb$. The permutation, $\pi(w)$ is then the union of a collection of partial one-to-one and order-preserving mappings, one for each member of $c(w)$. In this case $\pi = \pi_a \cup \pi_b$; the domain
and range of $\pi_a$ is defined respectively by the positions of the instances of the letter $a$ in $F(M)$ and $BW(M)$ respectively. Since $\pi_a$ is one-to-one and order-preserving, $\pi_a$ is defined uniquely by its domain and range, and of course $\pi_b$ is defined in the same fashion, and so on for any remaining letters in $c(w)$. In our example we obtain:

$$\pi(w) = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & 4 & 5 & 7 & 0 & 2 & 3 & 6 \end{pmatrix} = (014)(25)(376),$$

with $\text{dom } \pi_a = \{0, 1, 2, 3\}$ and $\text{dom } \pi_b = \{4, 5, 6, 7\}$. The cardinality of $M$ is equal to the number of cycles in the disjoint cycle representation of $\pi$, which here is 3. We may retrieve the Lyndon word of the multiset $M$ corresponding to each cycle of $\pi(w)$ by simply replacing each integer $m$ in the cycle by the letter $c \in A$ such that $m \in \text{dom } \pi_c$. In our case this means that we write $a$ whenever we see a number from 0 to 3 and we write $b$ otherwise. In this way we recover $M = \{aab, ab, abb\}$.

1.2 Establishing the transform through partial order-preserving mappings

Using Example 1.1 as a guide, we formally define the Burrows-Wheeler transform and explain its inversion.

**Definition 1.2.1 (Conjugation Map)** Let $\Pi : A^+ \to A^+$ be the mapping whereby $au \mapsto ua$ ($a \in A, u \in A^*$).

**Proposition 1.2.2** The Conjugation Map has the following properties:

(i) $\Pi$ is a permutation on $A^+$;

(ii) if $S \subseteq A^*$ is closed under conjugation then $\Pi|_S$ permutes $S$.

(iii) Suppose that $S \subseteq aA^n (a \in A, n \geq 0)$. Then $\Pi$ acts in an order-preserving manner on $S$.

(iv) For any word $w$ with root $(w) = r$, $|r|$ is the least positive integer $t$ such that $w \cdot \Pi^t = w$.

**Proof** (i) is clear from the definition and (ii) follows from (i) as the given
condition ensures that $S$ is closed under both $\Pi$ and $\Pi^{-1}$. To see (iii) suppose that $au \leq av$ with $au, av \in aA^n$. Since $|u| = |v|$, it follows that $u \leq v$ whence $ua \leq va$ and so $\Pi$ is order-preserving on the set $aA^n$. As for (iv), if $w \equiv xy$ then $w \cdot \Pi|x| = yx$ so in particular $w \cdot \Pi|[v] = w$. Suppose that $1 \leq |x| < |r|$ so that $r \equiv xx'$ say. Then $w' = w \cdot \Pi|x| \in x'xA^*$ and since $|x'| = |r|$ but $x'x \neq r$ as $r$ is primitive, it follows that $w' \neq w$. $
abla$

**Definitions 1.2.3** *(Burrows-Wheeler map)* Let $\mathcal{M}$ denote the set of all finite multisets of necklaces over $A$. Let $BW : \mathcal{M} \to A^*$ denote the Burrows-Wheeler map, the action of which is defined as follows. Take any $M \in \mathcal{M}$ so that $M = \{n_1, n_2, \ldots, n_t\}$ ($t \geq 0$) and let $l$ be the least common multiple of the lengths of the $n_i$. Sort by lexicographic order the collection $T = T(M)$ of powers $u^{n_i}$, where $u$ is a word of the necklace $n_i$. The table $T$ is then a dictionary of $n = |n_1| + |n_2| + \cdots + |n_t|$ words of common length $l$. The word $BW(M)$ is then the final column, read from top to bottom, of $T$. (Conventionally, $BW$ maps the empty set to the empty word.)

**Definition 1.2.4** *(Standard permutation of a word)* Let $w \in A^n$ and let $f(w)$ be the rearrangement of the letters of $w$ in lexicographic order. For each letter $a \in c(w)$ we define a partial one-to-one order-preserving mapping $\pi_a \in PIO_n$ through specifying dom $\pi_a$ and ran $\pi_a$ as follows: dom $\pi_a$ is the interval of length $|w|_a$ corresponding to the positions occupied by $a$ in $f(w)$ while ran $\pi_a$ is the set of positions occupied by $a$ in $w$. The standard permutation of $w$ is then $\pi = \bigcup_{a \in c(w)}\pi_a$.

**Remark 1.2.5** For any $i \in [n]$ there is a unique $a \in A$ such that $i \cdot \pi = i \cdot \pi_a$. For any $u \in A^*$, $u \equiv b_1b_2\cdots b_m$ we may define $\pi_u = \pi_{b_1}\pi_{b_2}\cdots \pi_{b_m}$. We note that $\pi_u \in PIO_n$ and for any $m \geq 1$ and $i \in [n]$ there is a unique word $u = u_{i,m}$ of length $m$ such that $i \cdot \pi_u$ is defined.

**Proposition 1.2.6** *[9, Proposition 10]* Let $M \in \mathcal{M}$ as in Definition 1.2.3, let the set of words that form the rows of $T(M)$ be denoted by $R(M)$ and let $u_i \in R(M)$ ($i \in [n]$). Let $\pi = \pi(w)$ be the standard permutation of $w = BW(M)$. Then the mapping $u_i \mapsto u_{i,\pi}$ is the restriction of the conjugation map $\Pi$ to $R(M)$.

**Proof** Suppose that $F(u_i) = a$ and that $u_i$ is the $j$th word of $R(M) \cap aA^*$. Then the $j$th instance of $a$ in the first column of $T(M)$ occurs in row $i$. Hence, regarded as intervals of $[n]$, dom $\Pi|_{R(M) \cap aA^*} = \text{dom} \pi_a$. Similarly,
since $w$ is the final column of $T(M)$, $\text{ran} \pi_a = R(M) \cap A^*a = (R(M) \cap aA^*)\Pi$. Therefore since $\pi_a$ and $\Pi|_{R(M) \cap aA^*}$ are order-preserving mappings (the latter by Proposition 1.2.2(iii)) with common domain and range, they are equal. Since this is true for all letters $a \in A$, we infer that $\pi = \Pi|_{R(M)}$ in that $i \mapsto i \cdot \pi$ if and only if $u_i \mapsto u_{i \cdot \pi}$ under $\Pi$. ■

The following was observed in [3], at least for the case of the BW transform of a single necklace.

**Proposition 1.2.7** Let $w = BW(M) \in A^n$, let $\pi = \pi(w)$ be the standard permutation and let $T(M) = (a_{ij})$. Then $a_{ij} = a_{i \cdot \pi,j - 1}$, which is to say that $\pi$ maps each column of $T(M)$ to its predecessor column modulo $l$, the number of columns of $T(M)$. In particular $\pi$ maps the first column of $T(M)$ to the last.

**Proof** Let $u_i$ be a row of $T(M)$ with $F(u_i) = b$ so that $u_i = bu$ say. Then by Proposition 1.2.6, $u_{i \cdot \pi} = ub$. The letter $a = a_{ij}$ will therefore be shifted one place back to appear in column $j - 1$ and in row $i \cdot \pi$ so that $a = a_{ij} = a_{i \cdot \pi,j - 1}$. ■

**Definition 1.2.8** (*Table of a word*) Let $w = b_0b_1 \cdots b_{n-1} \in A^+$ and let $\pi = \pi(w)$ be the standard permutation of $w$. Let us write the cycle $C_i = (i \ i \cdot \pi \ i \cdot \pi^2 \ \cdots \ i \cdot \pi^{r-1})$ so $r$ is least such that $i \cdot \pi^r = i$ and let $l$ denote the lcm of the cycle lengths. Define the table $T(w)$ to be the $n \times l$ table, the $i$th row of which is the unique word $u_i \in A^l$ such that $i \cdot \pi u_i$ is defined.

**Proposition 1.2.9** Let $w, \pi$ and $T(w)$ be as in Definition 1.2.8. Let $r = r(i)$ be the length of $C_i$ and let $x \in A^r$ be the corresponding prefix of $u = u(i)$, the $i$th row of $T(w)$. Then

(i) $x$ is the root of $u$;

(ii) all conjugates of $x$ arise as roots of the rows of $T(w)$ with multiplicity equal to that of $x$.

(iii) The rows of $T(w)$ are ranked lexicographically.

(iv) The final column of $T(w)$ is $w$.  

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Proof (i) By construction, \( i \cdot \pi^r = i \cdot \pi_x = i \) and \( x \) is the shortest prefix of \( u \) with this property. In particular, it follows from this that \( u = x^r \). To show that \( x \) is itself primitive, and so the root of \( u \), suppose to the contrary that \( x = y^t \) for some \( t \geq 2 \). Then \( i \cdot \pi_y \neq i \); without loss suppose that \( i < i \cdot \pi_y \). By applying \( \pi_y \) to both sides of this inequality (remembering that \( i \cdot \pi_y \) is defined for all \( s \leq t \)) we infer that

\[
i < i \cdot \pi_y < i \cdot \pi_y^2 < \cdots < i \cdot \pi_y^t = i \cdot \pi_x = i,
\]
a contradiction. Hence \( t = 1 \) and \( x \) is the root of \( u \), as claimed.

(ii) Let \( y = qp \) be a conjugate of \( x = pq \), the root of \( u(i) \). Then

\[
(i \cdot \pi_p) \cdot \pi_y = i \cdot \pi_{pq} = i \cdot \pi_{xp} = i \cdot \pi_x \pi_p = i \cdot \pi_p
\]

and since \( y \) is primitive, it follows that \( u(i \cdot \pi_p) = y^{[w]} \) and \( y \) is indeed the root of \( u(i \cdot \pi_p) \). This process associates each instance of the root \( x \) with an instance of the conjugate \( y \) in a one-to-one fashion, thereby matching the multiplicity of \( x \) to that of each of its conjugates \( y \) in the table \( T(w) \).

(iii) Let \( i < j \), let \( u = u(i) \) and \( v = v(j) \) be distinct words that occupy the respective rows \( i \) and \( j \) of \( T(w) \) and let \( p \in A^* \) be the longest common prefix of \( u \) and \( v \) so that \( u = pu_1 \) and \( v = pv_1 \) say. Then since \( \pi_p \) is order-preserving we have \( i_1 = i \cdot \pi_p < j \cdot \pi_p = j_1 \). Since \( u \) and \( v \) have common length \( l \), it follows that \( F(u_1) = a, F(v_1) = b \) say with \( a \neq b \). Moreover, since \( i_1 \in \text{dom } \pi_a, j_1 \in \text{dom } \pi_b \) and \( i_1 < j_1 \), it follows that \( a < b \) and so \( u < v \), as required.

(iv) Let \((a_{ij})\) denote the table \( T(w) \). Then \( a_{ij} = a \) if and only if \( i \cdot \pi^{j-1} \in \text{dom } \pi_a \). In particular, taking \( j = l \) gives that \( i \cdot \pi^{l-1} \in \text{dom } \pi_a \), whence \( i \cdot \pi^{-1} \in \text{dom } \pi_a \). At the same time we observe that \((w)_i = a\) exactly when \( i\pi^{-1} \in \text{dom } \pi_a \) and therefore \( a_{id} = (w)_i \) for all \( i \in [n] \), whence \( w \) is indeed the final column of \( T(w) \).

**Definition 1.2.10** (Inverse Burrows-Wheeler map) Define \( I : A^* \rightarrow \mathcal{M} \) as follows. Given \( w \in A^n \), form \( T(w) \) as in Definition 1.2.8. Let \( M = I(w) \) be the set of necklaces defined by the roots of the rows of \( T(w) \). (With \( \varepsilon \mapsto \emptyset \) under \( I \).)

**Theorem 1.2.11** [5, 8] The mapping \( I \) of Definition 1.2.10 is the inverse Burrows-Wheeler transform \( BW^{-1} : A^* \rightarrow \mathcal{M} \).
Proof We first prove that for any \( M \in \mathcal{M} \), \( I(BW(M)) = M \). Let \( T = T(M) \) be the table of \( M \) and let \( w = BW(M) \in A^n \) as in Definition 1.2.3. We show that the \( i \)th row \( u = u_i \) of \( T(M) \) is the \( i \)th row of \( T(w) \). By Proposition 1.2.6, identifying the rows of \( T(M) \) with the chain \([n]\) allows us to say that \( \pi(w) = \Pi|_{R(M)} \). In particular the lcm of the cycle lengths of both permutations is a common value \( l \), and by Proposition 1.2.2(iv) \( l \) is the lcm of the lengths of the roots of the words of \( R(M) \), so that \( T \) is an \( n \times l \) array.

Now suppose that \( u = av \ (a \in A) \). By Proposition 1.2.6 it follows that \( va = u_{i, \pi} = u_{i, \pi_a} \), so that \( i \cdot \pi = i \cdot \pi_a \). Repeated application of this observation gives that \( i \cdot \pi^l = i \cdot \pi_u \) so that \( u \) is the unique word of length \( l \) such that \( i \cdot \pi_u \) is defined. Hence \( T(M) = T(w) = T \) say. By Definition 1.2.10, \( I(w) \) is the set of necklaces formed by the roots of \( T \), which is the set \( M \) itself, and so \( I(BW(M)) = M \).

Conversely, take any \( w \in A^n \) say and let \( M = I(w) \). By Definition 1.2.10, \( M \) is the collection of necklaces of the roots of the rows of \( T(w) \). By Proposition 1.2.9(i), if \( x \) is the root of row \( i \) in \( T(w) \), then \( r = |x| \) is the length of the cycle \( C_i \) of \( \pi(w) \). It follows that there is a common value \( l \) for the lcm of the lengths of the roots of the rows of \( T(w) \) (which is the row length of \( T(M) \)) and the lcm of the cycle lengths of \( \pi(w) \) (which is the row length of \( T(w) \)). By Proposition 1.2.9(ii), all members of \( n(x) \) appear as roots of rows of \( T(w) \) with equal multiplicity while by (iii) the rows of \( T(w) \) are ranked lexicographically. It follows from all this that \( T(w) = T(M) = T \) is an \( n \times l \) array. Now \( BW(M) \) is the final column of \( T \), which by Proposition 1.2.9(iv) is the word \( w \). We conclude that \( BW(I(w)) = w \).  

Remark 1.2.12 The first part of the previous proof establishes that \( T(w(M)) = T(M) \) while the third paragraph shows that \( T(M(w)) = T(w) \) so that the bijection between words and necklaces is through equality of the corresponding table \( T \). Moreover Proposition 1.2.6 shows that the action of \( \Pi \) on \( R(T) \) corresponds to that of \( \pi(w) \) on \([n]\) and Proposition 1.2.7 shows that \( \pi \) acts to map each column of \( T \) onto its predecessor modulo \( l \).

Theorem 1.2.13 Let \( M \in \mathcal{M} \), \( T = T(M) \) and let \( i < j \) with \( u = u(i), v = u(j) \) two words in the set of rows \( R(M) \) of \( T \). Then \( u < r = \text{root}(v) \) if \( \text{root}(u) \) is Lyndon. In particular the Lyndon words appear in \( R(T) \) in lexicographic order.
Proof We prove the first statement by showing that if \( r \leq u(i) \) then \( \text{root}(u) \) is not Lyndon. Given this claim, suppose that \( \text{root}(u) \) and \( \text{root}(v) \) are both Lyndon words such that \( u < v \). Then \( \text{root}(u) \leq u < \text{root}(v) \) so that the Lyndon roots do indeed appear in lexicographic order in \( T \).

Since \( u < v \) with \( r = \text{root}(v) \leq u \) it follows that \( v \) is not primitive and so \( v = r^t \) for some \( t \geq 2 \). Since \( |u| = |v| \) and \( u < v \) we may write \( u = pax, v = pbq \) with \( a, b \in A, p, x, y \in A^* \) and \( a < b \). If \( |p| < |r| \), then \( r = pbq \) say whence \( u < r \), contrary to hypothesis and so \( |r| \leq |p| \) whence, since \( v \) is a power of \( r, p = r^ms \) for some maximal \( m \geq 1 \), and where \( s \in A^* \) is a prefix of \( r \). It follows that \( r = st \) where \( F(t) = b \) so that \( t = bw \) say \( (w \in A^* \) whence \( r = sbw \). Taking the factorization \( u = r^msax \), we see that \( u' = u \cdot r^m = sa(xr^m) \) is a conjugate of \( u \). We also have the factorization \( u = r^msax = sb(wr^{m-1}sx) \), whence \( u' < u \) as \( sa < sb \), which implies that \( \text{root}(u') < \text{root}(u) \) and so \( \text{root}(u) \) is not Lyndon, as required.

2 Semigroup of the Burrows-Wheeler transform

Semigroup of a necklace

In [6] the author wrote about the semigroup \( S(u) \) generated by the letters acting by conjugation on the necklace of a primitive word \( u \). In particular the question of when two words \( u \) and \( v \) have isomorphic semigroups \( S(u) \) and \( S(v) \) was settled by Theorem 2.4 of [6]. The semigroup \( S(u) \) is exactly the semigroup generated by the partial mappings \( \pi_a (a \in c(u)) \) encountered above. We show here that \( S(u) \) is isomorphic to the syntactic semigroup of the cyclic semigroup generated by the word \( u \).

We begin with a fixed primitive word \( u \in A^n \) over the finite ordered alphabet \( A = \{a_0 < a_1 < \cdots < a_{k-1}\} \). Consider the necklace \( n(u) = \{u_0 < u_1 < \cdots < u_{n-1}\} \), ordered lexicographically.

**Definition 2.1** Identify the chain \( n(u) \) with the chain \([n]\). The semigroup \( S(u) \) is the subsemigroup of \( \text{POI}_n \) generated by the set of \( k \) partial mappings \( \{\pi_a\} \) where \( \pi_{BW}(n(u)) = \cup_{i=0}^{k-1} \pi_{a_i} (a_i \in A) \).

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In this section it is convenient to denote the mapping \( \pi_a \) by \( a' \) so that the semigroup \( S(u) \) is generated by the set of partial mappings \( a' \) \((a \in A)\) where \( u_j \in \text{dom} \ a' \) if and only if \( F(u_j) = a \) so that \( u_j = ax \) say in which case \( (ax)a' = xa \in n(u) \). We write this using action notation as \( ax \cdot a = xa \), allowing us to suppress the dash to the right of the central dot without introducing ambiguity. The free monoid \( A^* \) acts on the right of \( n(u) \) in that \( u_j \cdot (xy) = (u_j \cdot x) \cdot y \) for all \( u_j \in n(u) \) and \( x, y \in A^* \) (taking \( \epsilon' \) to be the identity mapping). Note that \( S(u) \) depends only on the necklace \( n(u) \) and not its representative (and so we may assume that \( u = u_0 \), the Lyndon word of \( n(u) \), although this is not necessary). We make use of the following facts from Proposition 1.3 in [6]; part (iii) is well-known - see for example the text [7].

**Proposition 2.2** Let \( u = b_1 b_2 \cdots b_n \in A^+ \) and \( t \geq 0 \) be an integer. Let \( z = u^m b_1 b_2 \cdots b_s \) be the prefix of \( u^\omega \) of length \( t \) so that \( t = mn + s(0 \leq m, 0 \leq s \leq n - 1) \). Write \( v = b_1 b_2 \cdots b_s \) and define \( w \in A^+ \) by \( u = vw \). Then

(i) \( u \cdot v = wv \) and \( u \cdot u = u \);

(ii) \( z = u^m v \) is the unique word \( y \) of length \( t \) such that \( u \cdot y \) is defined.

(iii) A Lyndon word \( u \) has no border.

**Proof** (i) and (ii) are immediate consequences of the definition of the action of each letter on a given word. As for (iii), suppose to the contrary that \( u = xv \equiv vw \) for some \( x, v, w \in A^+ \). Then since \( u \) is Lyndon (and primitive) we may apply (i) to infer that \( u < u \cdot x \) and \( u < u \cdot v \). From the first of these inequalities we get \( u \cdot v < u \cdot xv \) as the latter is defined because \( u \cdot xv = u \cdot u = u \). However we then obtain \( u < u \cdot v < u \cdot xv = u \cdot u = u \), which is a contradiction. Therefore \( u \) has no border. ■

We now introduce a second realisation of \( S(u) \) via a certain syntactic congruence, thus producing \( S(u) \) without reference to mappings. (For background on syntactic semigroups and congruences see [11].) Let \( \langle u \rangle \) be the subsemigroup of \( A^+ \) of all positive powers of \( u \). Let \( \rho = \rho_u \) be the *syntactic congruence* on \( A^+ \) generated by \( \langle u \rangle \) so that for \( x, y \in A^+ \):

\[
x \rho y \iff (pxq \in \langle u \rangle \iff pyq \in \langle u \rangle \forall p, q \in A^*)
\]
Definition 2.3 The semigroup $S_u = A^+ / \rho_u$.

Lemma 2.4 Let $u \equiv vw$ and $u' \equiv vw$ be conjugate words. Then $S_u = S_{u'}$.

Proof Suppose that $(x, y) \in \rho_u$. Then for any $p, q \in A^+$ we have that if $pxq \equiv u^m \equiv (vw)^m$ for some $m \geq 1$ then $(wp)x(qv) \equiv w(vw)^m v \equiv (vw)^{m+1} \equiv u^{m+1}$. Since $(x, y) \in \rho_u$ this in turn implies that $(wp)y(qv) \equiv u^{r+1} \equiv (vw)^r \equiv u^r$. Hence it follows that $px \equiv u^r$ implies that $py \equiv (vw)^r$. Interchanging the roles of $x$ and $y$ in this argument yields the conclusion that $\rho_u \subseteq \rho_{u'}$ and by symmetry of the conjugation relation we see that the reverse inclusion also holds. Therefore $\rho_u = \rho_{u'}$ and $S_u = S_{u'}$. ■

Theorem 2.5 For any primitive word $u$, $S_u \cong S(u)$.

Proof For each $x \in A^+$, let $[x] = x\rho$ be the corresponding member of $S_u$ and $x'$ be that of $S(u)$. We show that a required isomorphism is given by the mapping $\theta : [x] \mapsto x'$. We first verify that $[x] = [y]$ if and only if $x' = y'$, thereby showing that $\theta$ is an injective function. It is then clear from the definition that $\theta$ is also surjective and $\theta$ is a homomorphism as for any $x, y \in A^+$ we then have

$$([x][y])\theta = [xy]\theta = (xy)' = x'y' = [x]\theta[y]\theta.$$ 

To this end suppose that $x\rho y$ and suppose further that $vw \in n(u)$, where $u = vw$ and that $vw \cdot x$ is defined. By Proposition 2.2(ii), $x \equiv (vw)^m c$ for some $m \geq 0$, where $vw \equiv cd$ say ($c, d \in A^*$). We shall show that $(vw) \cdot x = (vw) \cdot y$:

$$vw \cdot x = (vw) \cdot (vw)^m c = (vw) \cdot c = (cd) \cdot c = dc \in n(u)$$ \hspace{1cm} (2)

where the second and fourth equalities are by Proposition 2.2(i). Then since $vw \equiv cd$ we have:

$$wxdv \equiv w(vw)^m cdv \equiv (vw)^m w(vw)v \equiv (vw)^{m+2}$$

and so $wxdv \in \langle u \rangle$. Therefore since $x\rho y$ we infer that $wydv \equiv (vw)^r$ for some $r \geq 2 (r > 1$ as $y \neq \varepsilon$.) Hence, by cancelling $w$ on the left and $v$ on the right of this equation we obtain:

$$yd \equiv (vw)^{r-1}$$ \hspace{1cm} (3)
Invoking (2) and then (3) we infer that
\[ vw \cdot xd = (vw \cdot x) \cdot d = dc \cdot d = cd; \quad vw \cdot yd = vw \cdot (vw)^{r-1} = vw \equiv cd \quad (4) \]
Since the mapping \( d' \) is injective, (4) allows us to deduce that \( vw \cdot x = vw \cdot y \).
Since \( x, y \in A^+ \) were arbitrary, it follows that \( xpy \) implies that \( x' = y' \) as
the argument shows that for any \( u_i = vw \in n(u) \), if one of \( u_i \cdot x, u_i \cdot y \) is
defined, then both are defined and are equal.

To prove the converse we next suppose that for some \( x, y \in A^+ \), \( x' = y' \) and
suppose further that \( pxq \equiv u^m \) for some \( p, q \in A^* \) and \( m \geq 1 \). We
verify that \( pyq \in \langle u \rangle \). The following argument will hold with the roles of
\( x \) and \( y \) reversed and so this claim yields that if \( x' = y' \) then \( xpy \), thus
establishing that \( \theta \) is a one-to-one mapping from \( S_u \) into \( S(u) \). Since \( x' = y' \)
we obtain \( (u \cdot p) \cdot x = (u \cdot p) \cdot y \Rightarrow (u \cdot p) \cdot \cdot q = (u \cdot p) \cdot y \cdot q \Rightarrow u \cdot (pxq) = u \cdot (pyq) \Rightarrow u \cdot u^m = u \cdot (pyq) \); by Proposition 2.2(ii)
we infer that \( u = u \cdot pyq \). By Proposition 2.2(ii), \( pyq \equiv u^s v \) \((s \geq 0)\) for some non-empty prefix \( v \) of
\( u \equiv vw \) say. However then we obtain
\[ u \cdot pyq = u \cdot u^s v = u \cdot v = vw \cdot v = vw; \quad u \cdot pyq = u \equiv vw. \]
Hence \( u = vw \equiv vw \) and since \( u \) is primitive it follows that \( v \equiv u, w \equiv \varepsilon \) and
so \( pyq \equiv u^{s+1} \) for some \( s \geq 0 \). In particular, \( pyq \in \langle u \rangle \), as required to
complete the proof of the claim. Therefore \( \theta \) is an isomorphism from \( S_u \) to
\( S(u) \). □

For a multiset of necklaces \( M \), we may define the semigroup \( S(M) \) in
terms of the partial mappings of the standard permutation of \( BW(M) \).

**Theorem 2.6** Let \( M = \{ n_i = n(u_i) \} \) be a multiset of necklaces and
let \( n = |n_1| + |n_2| + \cdots + |n_t| \). Let \( S(M) \) be the subsemigroup of \( POI_n \)
generated by the set of mappings \( \{ \pi_a \} \) of \( \pi = \pi(BW(M)) \). Then \( S(M) \) is
a subsemigroup of \( POI_n \) isomorphic to a subdirect product of the syntactic
semigroups \( S_{u_i} \).

**Proof** Let \( C \) denote any member of the set of domains \( \{ C_1, C_2, \ldots, C_t \} \)
of disjoint cycles of \( \pi \). Since \( C \pi = C \) and each \( \pi_a \) is a restriction of \( \pi \),
it follows that \( \pi_a|_C \) is a (possibly empty) one-to-one and order-preserving
mapping in \( POI_C \), where \( C \) inherits a linear order as a subchain of \( [n] \).
The mapping whereby \( \pi_a \mapsto (\pi_a|_{C_1}, \pi_a|_{C_2}, \ldots, \pi_a|_{C_t}) \) induces an injective
homomorphism \( \phi : S(M) \to \Pi = POI_{C_1} \times POI_{C_2} \times \cdots \times POI_{C_t} \). Let \( p_j \)
denote the $j$th projection mapping on $\Pi$ so that $\phi p_j : S(M) \to POI_{C_j}$. We see that $S(u_i)$ is the image of $\phi p_j(i) : S(M) \to POI_{C_j(i)}$ (where $i \in \text{dom } C_j$) with generators $\pi_a|_{C_j(i)} (a \in c(u_i))$. It follows that $\phi$ may be regarded as an injective homomorphism of $S(M)$ into $S(u_1) \times S(u_2) \times \cdots \times S(u_t)$. Finally, by Theorem 2.5, $S(u_i) \cong S_{u_i}$, the syntactic semigroup of $\langle u_i \rangle$ and so we conclude that $S(M)$ is isomorphic to a subdirect product of the syntactic semigroups of each of the languages $\langle u_i \rangle$, as required. 

3 de Bruijn Words

In this section we take our alphabet to be $A = \{0 < 1 < \cdots < k - 1\}$ ($k \geq 2$), although we continue to refer to its members $a \in A$ as letters. An interesting special case is where we take the BW transform of (the necklace of) a de Bruijn word of span $n$ over a finite $k$-ary alphabet, which can be defined as a word $w$ of length $k^n$ for which every word of length $n$ appears exactly once as a cyclic factor of $w$. For every $n$ and for every $k$-ary alphabet $A$, de Bruijn words $d_n$ exist and their number is $\frac{(k)!}{k^{n-1}}$ [1].

Definition 3.1 A multiset $M$ of necklaces $\{n_i\}$ is a de Bruijn set of span $n$ over $A$ if $|n_1| + |n_2| + \cdots + |n_t| = k^n$ and every $w \in A^n$ is a prefix of some power of some word of the necklaces $n_i$.

Remarks 3.2 The number of distinct prefixes of length $n$ of powers of the words of the necklaces $n_i$ is at most $k^n$ so, given that $M$ is a de Bruijn set of span $n$, every word in $A^n$ can be read exactly once within the necklaces of $M$. It also follows in particular that no two necklaces in $M$ are equal so that $M$ is indeed a set, as opposed to a multiset, of necklaces.

Lemma 3.3 Let $M$ be a de Bruijn set of span $n$. Then $M$ contains a necklace of length at least $n$.

Proof There exist Lyndon words $u$ of length $n$ (eg. take $u = ab^n-1$, where $a < b$). Let $n_i \in M$ be a necklace of cardinal $m < n$ so that $n = tm + l$ say with $0 \leq l \leq m - 1$. Any prefix of length $n$ of a power factor of a word $v \in n_i$ has a border of length $l$ if $l \neq 0$ and has a border of length $m$ otherwise. Since $u$ is a Lyndon word, $u$ has no border by Proposition 2.2(iii), and so $u$ cannot arise as a prefix power of a word $v \in n_i$. Since $u$ is a prefix power of
some word in some necklace of \( M \), it follows that \( M \) contains a necklace of cardinal at least \( n \). ■

The bound of \( n \) in Lemma 3.3 is tight: see Theorem 3.8 below. It follows from Lemma 3.3 that the length \( l \) of the rows of the table \( T = T(M) \) is at least \( n \). Consider the sub-table consisting of the first \( n \) columns of \( T \). Since \( M \) is an \( n \) span de Bruijn set, the rows of this sub-table form the dictionary of \( A^n \). Each \( u \in A^n \) is the prefix of \( k \) successive rows of \( T \) and if two of these rows ended with the same letter \( a \in A \), then the images of these two rows under \( \Pi \) would both begin with \( au \), from which it would follow that \( au \in A^n \) would be a prefix of a power of two distinct words of the necklaces of \( M \), contrary to \( M \) being a de Bruijn set of span \( n \). It follows that the final column of \( T \) is a product of \( k^{n-1} \) members (possibly with repetitions) taken from the set \( G \) consisting of all \( k! \) products of distinct members of \( A \). These observations establish the forward implication in the following result.

**Theorem 3.4** The set of all BW transforms of de Bruijn sets \( M \) of span \( n \) over a \( k \)-letter alphabet is \( \Gamma_{k,n} = G^{k^{n-1}} \).

**Examples 3.5** Let \( k = 2, n = 4 \). We may write \( A = \{a < b\} \) so that \( G = \{\alpha, \beta\} \) where \( \alpha = ab, \beta = ba \). Take \( v = \beta^4\alpha^3 \in G^{k^{n-1}} = G^8 \). The standard permutation \( \pi(v) \) is the transitive cycle

\[
\pi(v) = (0 1 3 7 15 14 12 9 2 5 11 6 13 10 4 8),
\]
yielding the span 4 Lyndon de Bruijn word \( w = aaaa bbbb aaba bbab \). As a second example take \( v = \beta^2\alpha^2\beta^2\alpha^2 \beta \) so that

\[
\pi(v) = (0 1 2 4 9 3 7 15 14 13 11 6 12 8)(5 10);
\]
the corresponding set of Lyndon words is \( \{aaaabaabbbabbb, ab\} \), the cyclic 4-factors of which are all the \( 2^4 = 16 \) words of \( A^4 \) with \( \{abab, bab\} \) arising from the necklace defined by the Lyndon word \( ab \).

We prove the reverse implication in Theorem 3.4 via two lemmas.

**Lemma 3.6** Let \( v \in \Gamma_{k,n} \). Then \( \pi(v) = \pi = \bigsqcup_{i=0}^{i=k-1} \pi_i \), a union of \( k \) order preserving partial mappings with \( \text{dom} \ \pi_i = \{x = \varepsilon_1\varepsilon_2\cdots\varepsilon_n \in [k^n] : \varepsilon_1 = i\} \) for \( 0 \leq i \leq k - 1 \). The sets \( \pi_i \) also partition \([k^n]\) and each range set
is itself a transversal of the partition of \([k^n]\) into the successive intervals of length \(k\) which are:

\[
[jk, (j+1)k - 1], \quad 0 \leq j \leq k^{n-1} - 1
\]

\((5)\)

**Proof** The description of the sets \(\text{dom } \pi_i\) follows from the fact that \(|v|_i\) is the same value, \(k^{n-1}\), for each \(i\) \((0 \leq i \leq k-1)\) and the sets \(\text{ran } \pi_i\) always partition the base set as \(\pi\) is a permutation. The claim as regard transversals follows as each \(v \in \Gamma_{k,n}\) is a product of words from \(G\).

For any \(x \in [k^n]\) and integer \(m \geq 0\) there is a unique product \(p = p_{x,m} = \pi_{\varepsilon_1}\pi_{\varepsilon_2} \cdots \pi_{\varepsilon_m}\) with each \(\varepsilon_i \in [k]\), such that \(x \cdot p\) is defined. The product \(p_{x,m}\) can therefore be identified with \(\varepsilon_1\varepsilon_2 \cdots \varepsilon_m\), which we shall call the \(m\)-string of \(x\).

**Lemma 3.7** Let \(e = \varepsilon_1\varepsilon_2 \cdots \varepsilon_m\) be an \(m\)-digit \(k\)-ary expression \((1 \leq \varepsilon_m \leq n)\). Then for any \(x \in [k^n]\) whose \(n\)-digit \(k\)-ary representation has \(e\) as a prefix, the \(k\)-ary \(m\)-string of \(x\) is \(e\) in the standard permutation \(\pi(v)\), for every \(v \in \Gamma_{k,n}\). Moreover, the domain of the partial mapping \(p_e = \pi_{\varepsilon_1}\pi_{\varepsilon_2} \cdots \pi_{\varepsilon_m}\) is the interval of all \(x\), the \(k\)-ary representation of which begins with \(e\). In particular, \(\text{dom } p_e = \{x\}\).

**Proof** By Lemma 3.6, \(x \cdot \pi_i\) is defined if and only if \(F(x) = i\) and so the claim holds if \(m = 1\). We shall now verify that \(x \cdot \pi_{\varepsilon_1}\) has the \(k\)-ary form \(\varepsilon_2\varepsilon_3 \cdots \varepsilon_n\varepsilon'_1\), \((\varepsilon'_1 \in [k])\), from which the result follows by repeated application of this fact. Now since \(\pi_{\varepsilon_1}\) is order-preserving, it follows from Lemma 3.6 that we may identify the interval of \((5)\) in which \(x \cdot \pi_{\varepsilon_1}\) lies by putting \(j = \varepsilon_2\varepsilon_3 \cdots \varepsilon_n\), giving:

\[
[\varepsilon_2\varepsilon_3 \cdots \varepsilon_n k, (\varepsilon_2\varepsilon_3 \cdots \varepsilon_n + 1)k - 1] = \varepsilon_2\varepsilon_3 \cdots \varepsilon_n 0, \varepsilon_2\varepsilon_3 \cdots \varepsilon_n 0 + (k - 1)
\]

and so \(x \cdot \pi_{\varepsilon_1} = \varepsilon_2\varepsilon_3 \cdots \varepsilon_n\varepsilon'_1\), as required. By what we have just proved and the uniqueness of the products \(p_{x,m}\), the integer \(x \in \text{dom } p_e\) if and only if \(e\) is a prefix of \(x\), whence the final claim follows.

**Proof of Theorem 3.4.** The forward implication was proved in the preamble to the theorem so consider the converse. For \(v \in \Gamma_{k,n}\) consider \(M = BW^{-1}(v)\). By Lemma 3.7, for any \(x \in [k^n]\), \(u = x\) is the unique word \(u \in A^n\) such that \(x \cdot \pi_u\) is defined. Since some members \(x \in [k^n]\) such as
\( x = 1 \), are primitive, the table \( T(M) = T(v) \) has at least \( n \) columns. It follows that the prefix of length \( n \) of the row \( x \) of \( T(v) \) is \( x \) and so the sub-table of the first \( n \) columns of \( T(v) \) has as its rows the members of \( [k^n] \) written in numerical order. In particular \( x \) occurs among the \( k^n \) factors of length \( n \) that can be read from the \( k^n \) words of the necklaces of \( M \), and so each such \( x \) must occur exactly once and therefore \( M \) is a de Bruijn set of span \( n \). 

We next look at the special case where \( v \) is a power of \( \alpha = 1^2 \cdot \cdot \cdot (k-1) \).

**Theorem 3.8** Let \( v = \alpha^{kn-1} \), let \( M = BW^{-1}(v) \) and let \( T = T(v) = T(M) \). Then the rows of \( T \) are simply the list of numbers \( [kn] \). Moreover \( BW^{-1}(v) \) is the set of necklaces of Lyndon words of length dividing \( n \). The Lyndon words of the roots of the necklaces of \( M \) occur in the rows of \( T \) in lexicographic order.

**Proof** As in the proof of Theorem 3.4, we see that the sub-table of the first \( n \) columns of \( T \) simply lists the numbers of \( [kn] \). However since \( v = \alpha^{kn-1} \), for \( x = \varepsilon_1\varepsilon_2\cdots \varepsilon_n, x \cdot \pi_1 \) is the \( \varepsilon_1 \)th member \( (0 \leq \varepsilon_1 \leq k-1) \) of the specified interval in (5), that is to say, \( x\pi_1 = \varepsilon_2\varepsilon_3\cdots \varepsilon_n\varepsilon_1 \); by repetition of this observation we infer that for any \( x = \varepsilon_1\varepsilon_2\cdots \varepsilon_n \), the sequence \( x \cdot \pi, x \cdot \pi^2, \cdots x \cdot \pi^{n-1} \) (where \( \pi = \pi(v) \)) is the cyclic sequence under \( \Pi \) of \( x = \varepsilon_1\varepsilon_2\cdots \varepsilon_n \). Since \( x \cdot \pi^n = x \), it follows that the cardinal of the corresponding necklace is a divisor of \( n \); in particular \( l \), the lcm of the length of the roots of words of the rows is \( n \), so that \( T \) is simply the table of \( [kn] \). The least member of each necklace is by definition a Lyndon word. Every Lyndon word \( w \) of length dividing \( n \) has a power which is some word \( x \in [kn] \) and so \( w \) occurs as a Lyndon word of some necklace in \( BW^{-1}(v) \). The Lyndon roots of the words of \( T \) occur in lexicographic order by Theorem 1.2.13.

**Example 3.9** Let us take \( k = 2, n = 5 \), and again reverting to the alphabet \( A = \{a < b\} \), we have \( \alpha = ab \) and \( v = \alpha^{24} = (ab)^{16} \). Then

\[
\pi(v) = (0)(1\ 2\ 4\ 8\ 16)(3\ 6\ 12\ 24\ 17)(5\ 10\ 20\ 9\ 18)(7\ 14\ 28\ 25\ 19)
\]

\[
(11\ 22\ 13\ 26\ 21)(15\ 30\ 29\ 27\ 23)(31).
\]

Expressed as a concatenation of Lyndon words of the corresponding necklaces we obtain:

\[
BW^{-1}(v) = a \cdot aaaaab \cdot aaabb \cdot aabab \cdot aabbb \cdot ababb \cdot abbbb \cdot b.
\]
This is indeed the first de Bruijn word of span 5 in the lexicographic order. That this is always the case is a well-known theorem of Frederickson and Maiorana. (See also [10] for an alternative proof.)

**Theorem 3.10** [4] For a given $n$, the lexicographic concatenation of all Lyndon words of length dividing $n$ is the de Bruijn word of span $n$ that lies first in the lexicographic order.

**Corollary 3.11** Taken in ascending order of their Lyndon words, the concatenation of the Lyndon words of the necklaces of $BW^{-1}(\alpha^{k^{n-1}})$ is the first de Bruijn word of span $n$ in the lexicographic order.

**Example 3.12** Let us take $k = n = 3$ so that $\alpha = abc$ say and calculate $BW^{-1}(v)$ where $v = \alpha^{k^{n-1}} = (abc)^9$. We find that

$$\pi_v = (0)(139)(2618)(41210)(51519)(72111)
\quad (82420)(13)(141622)(172523)(26);$$

and so the least de Bruijn word that contains all words of length 3 over the alphabet $A = \{a < b < c\}$ as its set of cyclic factors is the following concatenation of Lyndon words of lengths 1 or 3 over $A$:

$$BW^{-1}(\alpha^9) = a \cdot aab \cdot aac \cdot abb \cdot abc \cdot acb \cdot acc \cdot b \cdot bbc \cdot bcc \cdot c.$$

### 4 Maximum number of distinct factors of a word

As an application of de Bruijn words we derive the functional form for the maximum number of distinct factors in $A^+$ of a word of length $n$ over a fixed finite alphabet $A$. The upper bound in our result comes from observing that long words must have repeated short factors while the proof for the lower bound relies on the fact that factors of de Bruijn words have no repeats of their long factors. The topic of the number of subwords of a word has been extensively investigated: for example see Section 6.3 of [7].

Consider the finite alphabet $A = A_k = \{a_1, a_2, \ldots, a_k\}$. The set $A^{\leq m} = \{w : w \in A^+ \text{ and } |w| \leq m\}$. The number of distinct factors of $w$ will be denoted by $f_w$. 

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Lemma 4.1 With repeats, the number of factors in \( A^+ \) of \( w \in A^n \) \((n \geq 1)\) is \( \frac{1}{2} n(n+1) \).

Proof A factor of \( w \) is determined by the choice of two distinct positions with each position occurring either between letters or at either end of \( w \). There are \( \binom{n+1}{2} = \frac{1}{2} n(n+1) \) such pairs. \( \blacksquare \)

Corollary 4.2 For \( w \in A^n \) \((n \geq 1)\) we have \( n \leq f_w \leq \frac{1}{2} n(n+1) \). Moreover, the lower bound is obtained if and only if \( |c(w)| = 1 \) and the upper bound is attained if and only if \( n \leq k \).

Proof The upper bound for \( f_w \) comes from Lemma 4.1. Since any word \( w \in A^n \) has \( n \) distinct prefixes it follows that \( n \leq f_w \) always holds. If \( |c(w)| = 1 \), then \( w = a^n \) for some \( a \in A \) and the set of factors of \( w \) is \( \{a^t : 1 \leq t \leq n\} \) and is of cardinal \( n \). On the other hand if \( |c(w)| \geq 2 \) then, in addition to its \( n \) prefixes, \( w \) also has the factor \( b \in A \) where \( b \neq F(w) \) so that \( n < f_w \). Next suppose that \( n \leq k \). Put \( w = a_1a_2\cdots a_n \); no two factors of \( w \) have the same content so the factors of \( w \) are pairwise distinct, showing that the upper bound in the statement is attained in this case. For all remaining cases we have \( 2 \leq k < n \) in which instance \( w \) has two identical 1-factors and so \( f_w < \frac{1}{2} n(n+1) \). \( \blacksquare \)

In light of Corollary 4.2 we shall henceforth assume that \( 2 \leq k < n \).

Definition 4.3 Let \( f(n) = \max \{f_w : w \in A^n\} \).

Theorem 4.4 \( \frac{1}{2} n^2 - f(n) = O(n \log n) \).

Proof For \( 1 \leq r \leq n \), a word \( w \in A^n \) has \( n - r + 1 \) (not necessarily distinct) \( r \)-factors and \( |A^r| = k^r \). Hence there are at least \( n - r + 1 - k^r \) repeated \( r \)-factors in \( w \). Let \( t \) be the greatest value of \( r \) such that \( r + k^r \leq n \), noting that \( 1 \leq t \). The total number of repeated factors in \( w \) is then at least:

\[
\sum_{r=1}^{t} (n - r + 1 - k^r) = (n + 1)t - \frac{1}{2}t(t + 1) - k \frac{k^t - 1}{k - 1} \quad (6)
\]

Now since \( t + k^t \leq n < t + 1 + k^{t+1} \) we have \( n < 2k^{t+1} \); by taking logarithms to the base \( k \) we obtain \( t < \log_k n < (1 + \log_k 2) + t \) so that \( t = O(\log n) \).
Moreover, \( k^t = O(n) \) whence it follows that
\[
f(n) \leq \frac{1}{2} n(n+1) - (n+1)O(\log n) + \frac{1}{2} (O(\log n))^2 + O(n) = \frac{1}{2} n^2 - O(n \log n)
\]  \hspace{1cm} (7)

Conversely, given \( n \), let \( m \geq 1 \) be determined by the inequalities \( k^{m-1} < n \leq k^m \). Take \( w \in A^n \) to be a factor of a de Bruijn word \( d = d_m \) of span \( m \) over \( A \). For any positive integer \( p \leq n \) there are \( n - p + 1 \) factors of length \( p \) in \( w \). Moreover if \( m \leq p \), these factors are pairwise distinct as the members of the set of prefixes of length \( m \) of these factors are pairwise distinct since \( d \) is a de Bruijn word of index \( m \). Hence
\[
f_w \geq 1 + 2 + \cdots + (n-m+1)
\]
\[
\Rightarrow f_w \geq \frac{1}{2} (n-m+1)(n-m+2) = \frac{1}{2} n^2 - nm - \frac{1}{2} (3(n-m)+m^2)+1 > \frac{1}{2} n^2 - nm
\]  \hspace{1cm} (8)

Now we have \( k^{m-1} < n \leq k^m \), whence \( m = O(\log n) \) and so (8) yields:
\[
f(n) \geq f_w \geq \frac{1}{2} n^2 - O(n \log n)
\]  \hspace{1cm} (9)

Combining (7) and (9) we conclude that \( \frac{1}{2} n^2 - f(n) = O(n \log n) \).  \hspace{1cm} \Box

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