CLUSTERING WORDS

SÉBASTIEN FERENCZI AND LUCA Q. ZAMBONI

ABSTRACT. We characterize words which cluster under the Burrows-Wheeler transform as those words $w$ such that $ww$ occurs in a trajectory of an interval exchange transformation, and build examples of clustering words.

In 1994 Michael Burrows and David Wheeler [1] introduced a transformation on words which proved very powerful in data compression. The aim of the present note is to characterize those words which cluster under the Burrows-Wheeler transform, that is to say which are transformed into such expressions as $4^a3^b2^c1^d$ or $2^a5^b3^c1^d4^e$. Clustering words on a binary alphabet have already been extensively studied (see for instance in [8, 11]) and identified as particular factors of the Sturmian words. Some generalizations to $r$ letters appear in [11], but it had not yet been observed that clustering words are intrinsically related to interval exchange transformations (see Definitions 1 and 2 below). This link comes essentially from the fact that the array of conjugates used to define the Burrows-Wheeler transform gives rise to a discrete interval exchange transformation sending its first column to its last column. It turns out that the converse is also true: interval exchange transformations generate clustering words. Indeed we prove that clustering words are exactly those words $w$ such that $ww$ occurs in a trajectory of an interval exchange transformation. On a binary letter alphabet, this condition amounts to saying that $ww$ is a factor of an infinite Sturmian word.

We end the paper by some examples and questions on how to generate clustering words.

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1. DEFINITIONS

Let $A = \{a_1 < a_2 < \cdots < a_r\}$ be an ordered alphabet and $w = w_1 \cdots w_n$ a primitive word on the alphabet $A$, i.e. $w$ is not a power of another word. For simplification we suppose that each letter of $A$ occurs in $w$.

The Parikh vector of $w$ is the integer vector $(n_1, \ldots, n_k)$ where $n_i$ is the number of occurrences of $a_i$ in $w$. The (cyclic) conjugates of $w$ are the words $w_i \cdots w_n w_1 \cdots w_{i-1}$, $1 \leq i \leq n$. As $w$ is primitive, $w$ has precisely $n$-cyclic conjugates. Let $w_{i,1} w_{i,2} \cdots w_{i,n}$ denote the $i$-th conjugate of $w$ where the $n$-conjugates of $w$ are ordered in ascending lexicographical order. Then the Burrows-Wheeler transform of $w$, denoted by $B(w)$, is the word $w_{1,n} w_{2,n} \cdots w_{n,n}$. In other words, $B(w)$ is obtained from $w$ by first ordering its cyclic conjugates in ascending order in a rectangular array, and then reading off the last column. We say $w$ is $\pi$-clustering if $B(w) = a_{\pi 1}^{n_1} \cdots a_{\pi r}^{n_r}$, where

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\( \pi \neq Id \) is a permutation on \( \{1, \ldots, r\} \). We say \( w \) is perfectly clustering if it is \( \pi \)-clustering for \( \pi i = r + 1 - i, 1 \leq i \leq r \).

**Definition 1.** A (continuous) \( r \)-interval exchange transformation \( T \) with probability vector \((\alpha_1, \alpha_2, \ldots, \alpha_r)\), and permutation \( \pi \) is defined on the interval \([0, 1]\), partitioned into \( r \) intervals

\[
\Delta_i = \left[ \sum_{j<i} \alpha_j, \sum_{j \leq i} \alpha_j \right],
\]

by

\[
Tx = x + \tau_i \quad \text{when} \quad x \in \Delta_i,
\]

where \( \tau_i = \sum_{\pi^{-1}(j)<\pi^{-1}(i)} \alpha_j - \sum_{j<i} \alpha_j \).

Intuitively this means that the intervals \( \Delta_i \) are re-ordered by \( T \) following the permutation \( \pi \). We refer the reader to [13] which constitutes a classical course on general interval exchange transformations and contains many of the technical terms found in Section 3 below. Note that our use of the word “continuous” does not imply that \( T \) is a continuous map on \([0, 1]\) (though it can be modified to be made so); it is there to emphasize the difference with its discrete analogous.

**Definition 2.** A discrete \( r \)-interval exchange transformation \( T \) with length vector \((n_1, n_2, \ldots, n_r)\), and permutation \( \pi \) is defined on a set of \( n_1 + \cdots + n_r \) points \( x_1, \ldots, x_{n_1+\cdots+n_r} \) partitioned into \( r \) intervals

\[
\Delta_i = \{ x_k, \sum_{j<i} n_j < k \leq \sum_{j \leq i} n_j \}
\]

by

\[
Tx_k = x_{k+s_i} \quad \text{when} \quad x_k \in \Delta_i,
\]

where \( s_i = \sum_{\pi^{-1}(j)<\pi^{-1}(i)} n_j - \sum_{j<i} n_j \).

We recall the following notions, defined for any transformation \( T \) on a set \( X \) equipped with a partition \( \Delta_i, 1 \leq i \leq r \).

**Definition 3.** The trajectory of a point \( x \) under \( T \) is the infinite sequence \( (x_n)_{n \in \mathbb{N}} \) defined by \( x_n = i \) if \( T^n x \) belongs to \( \Delta_i, 1 \leq i \leq r \). The mapping \( T \) is minimal if whenever \( E \) is a nonempty closed subset of \( X \) and \( T^{-1} E = E \), then \( E = X \).

2. **Main result**

**Theorem 1.** Let \( w = w_1 \cdots w_n \) be a primitive word on \( A = \{1, \ldots, r\} \), such that every letter of \( A \) occurs in \( w \). The following are equivalent:

1. \( w \) is \( \pi \)-clustering,
2. \( ww \) occurs in a trajectory of a minimal discrete \( r \)-interval exchange transformation with permutation \( \pi \),
3. \( ww \) occurs in a trajectory of a discrete \( r \)-interval exchange transformation with permutation \( \pi \),
4. \( ww \) occurs in a trajectory of a continuous \( r \)-interval exchange transformation with permutation \( \pi \).
Proof. ((2), (3) or (4) implies (1)) By assumption there exists a point $x$ whose initial trajectory of length $2n$ is the word $ww$. Consider the set $E = \{Tx, T^2x, \ldots, T^n x\}$. Then for each $y \in E$, the initial trajectory of $y$ of length $n$, denoted $O(y)$, is a cyclic conjugate of $w$.

Suppose $y$ and $z$ are in $E$, and $y$ is to the left of $z$ (meaning $y < z$). Let $j$ be the smallest nonnegative integer such that $T^j y$ and $T^j z$ are not in the same $\Delta_i$. Then $T^j y$ is to the left of $T^j z$, either because $j = 0$ or because $T$ is increasing on each $\Delta_i$. Thus $O(y)$ is lexicographically smaller than $O(z)$.

Thus $B(w)$ is obtained from the last letter $l(y)$ of $O(y)$ where the points $y$ are ordered from left to right. But $l(y)$ is the label of the interval $\Delta_i$, where $T^{n-1} y$, or equivalently $T^{-1} y$, falls. Thus by definition of $T$, if $y$ is to the left of $z$ then $\pi^{-1}(l(y)) \leq \pi^{-1}(l(z))$, and if $y'$ is between $y$ and $z$ with $l(y) = l(z)$, then $l(y') = l(y) = l(z)$, hence the claimed result.

Proof. ((2) implies (3) implies (4)) The first implication is trivial. The second follows from the fact that the trajectories of the discrete $r$-interval exchange transformation with length vector $(n_1, n_2, \ldots, n_r)$, and permutation $\pi$, and of the continuous $r$-interval exchange transformation with probability vector $(2/n_1 + \cdots + n_r, \ldots, 2/n_1 + \cdots + n_r)$ and permutation $\pi$ are the same. We note that this continuous interval exchange transformation is never minimal, while the discrete one may be.

We now turn to the proof of the converse, which uses a succession of lemmas. Throughout this proof, unless otherwise stated, a given word $w$ is a primitive word on $\{1, \ldots, r\}$, and every letter of $\{1, \ldots, r\}$ occurs in $w$; $(n_1, \ldots, n_r)$ is its Parikh vector, the $w_{1,1} \cdots w_{1,n}$ are its conjugates.

The first lemma states that $B$ is injective on the conjugacy classes, which is proved for example in [2] or [12]; we give here a short proof for sake of completeness.

**Lemma 2.** Every antecedent of $B(w)$ by the Burrows-Wheeler transform is conjugate to $w$.

**Proof.** In the array of the conjugates of $w$, each column word $w_{1,j} \cdots w_{n,j}$ has the same Parikh vector as $w$, so we retrieve this vector from $B(w)$; thus we know the first column word, which is $1^{n_1} \cdots r^{n_r}$, and the last column word which is $B(w)$. Then the words $w_{n,j} w_{1,j}$ are precisely all words of length 2 occurring in the conjugates of $w$, and by ordering them we get the first two columns of the array. Then $w_{n,j} w_{1,j} w_{2,j}$ constitute all words of length 3 occurring in the conjugates of $w$, and we get also the subsequent column, and so on until we have retrieved the whole array, thus $w$ up to conjugacy.

It is easy to see that $B$, viewed as a mapping from words to words, is not surjective (see for instance [12]). A more precise result will be proved in Corollary 4 below.

**Lemma 3.** If $w$ is $\pi$-clustering, the mapping $w_{1,j} \mapsto w_{n,j}$ defines a discrete $r$-interval exchange transformation with length vector $(n_1, n_2, \ldots, n_r)$, and permutation $\pi$.

**Proof.** We order the occurrences of each letter in $w$ by putting $w_i < w_j$ if the conjugate $w_i \cdots w_n w_1 \cdots w_{i-1}$ is lexicographically smaller than $w_j \cdots w_n w_1 \cdots w_{j-1}$. By primitivity, the $n$ letters of $w$ are uniquely ordered as

$$1_1 < \cdots < 1_{n_1} < 2_1 < \cdots < 2_{n_2} < \cdots < r_1 < \cdots < r_{n_r},$$

and the first column word is $1_1 \cdots 1_{n_1} 2_1 \cdots 2_{n_2} \cdots r_1 \cdots r_{n_r}$. We look at the last column word: if $w_{n,j}$ and $w_{n,j+1}$ are both some letter $k$, the order between these two occurrences of $k$ is given by the next letter in the conjugates of $w$, and these are respectively $w_{1,j}$ and $w_{1,j+1}$. Thus $w_{n,j} < w_{n,j+1}$. Together with the hypothesis, this implies that the last column word is

$$(\pi_1)_1 \cdots (\pi_1)_{n_{\pi_1}} \cdots (\pi_r)_1 \cdots (\pi_r)_{n_{\pi_r}}.$$
Thus, if we regard the rule \( w_{1,j} \mapsto w_{n,j} \) as a mapping on the \( n_1 + \ldots + n_r \) points 
\[
\{1, \ldots, 1_{n_1}, 2_1, \ldots 2_{n_2}, \ldots, r_1, \ldots, r_{n_r}\}
\]
and put \( \Delta_i = \{i_1, \ldots, i_{n_i}\} \), we get the claimed result. \( \square \)

**Corollary 4.** If the discrete \( r \)-interval exchange transformation \( T \) with length vector \( (n_1, n_2, \ldots, n_r) \), and permutation \( \pi \) is not minimal, the word \((\pi 1)^{n_{r-1}} \cdots (\pi r)^{n_r}\) has no primitive antecedent by the Burrows-Wheeler transform.

*Proof.* Let \( w \) be such an antecedent. By the previous lemma, the map \( w_{1,j} \mapsto w_{n,j} \) corresponds to \( T \). If \( T \) is not minimal, there is a proper subset \( E \) of \( \{1, \ldots, 1_{n_1}, 2_1, \ldots 2_{n_2}, \ldots, r_1, \ldots, r_{n_r}\} \) which is invariant by \( w_{1,j} \mapsto w_{n,j} \). Thus, in the conjugates of \( w \), preceding any occurrence of a letter of \( E \) is another occurrence of a letter of \( E \). This implies that \( w \) is made up entirely of letters of \( E \), a contradiction. \( \square \)

*Proof.* ((1 implies (2)) Let \( w \) be as in the hypothesis. Then \( B(w) = (\pi 1)^{n_{r-1}} \cdots (\pi r)^{n_r} \). Thus the transformation \( T \) of Lemma 1 is minimal, and thus has a periodic trajectory \( w'w'w' \ldots \), where \( w' \) has Parikh vector \((n_1, \ldots, n_r)\). If \( w' = w^k \), then \( n_i = kn'_i \) for all \( i \), and the set made with the \( n'_i \) leftmost points of each \( \Delta_i \) is \( T \)-invariant, thus \( w' \) must be primitive.

By the proof, made above, that (2) implies (1), \( w' \) is \( \pi' \)-clustering. Hence \( B(w') = B(w) \) and, by Lemma 1, \( w \) is conjugate to \( w' \), hence \( ww \) occurs in a trajectory of \( T \). \( \square \)

Some of the hypotheses of Theorem II may be weakened.

**Alphabet.** \( \{1, \ldots, r\} \) can be replaced by any ordered set \( A = \{a_1 < a_2 < \cdots < a_r\} \) by using a letter-to-letter morphism. Thus for a given word \( w \), we can restrict the alphabet to the letters occurring in \( w \). Note that if \( ww \) occurs in a trajectory of an \( r \)-interval exchange transformation, but only the letters \( j_1, \ldots, j_d \) occur in \( w \), then, by the reasoning of the proof that (4) implies (1), \( w \) is \( \pi' \)-clustering, where \( \pi' \) is the unique permutation on \( \{1, \ldots, d\} \) such that \((\pi')^{-1}(y) < (\pi')^{-1}(z) \) iff \( \pi^{-1}(j_y) < \pi^{-1}(j_z) \). If \( \pi \) is a permutation defining perfect clustering, then so is \( \pi' \).

**Primitivity.** The Burrows-Wheeler transformation can be extended to a non-primitive word \( w_1 \cdots w_n \), by ordering its \( n \) (non necessarily different) conjugates \( w_i \cdots w_n w_1 \cdots w_{i-1} \) by non-strictly increasing lexicographical order and taking the word made by their last letters.

In this case the result of Lemma 4 does not extend: For example \( B(1322313223) = 3333222211 \) though the discrete 3-interval exchange transformation with length vector \((2, 2, 4)\), and permutation \( \pi 1 = 3, \pi 2 = 2, \pi 3 = 1 \) is not minimal. Note that if \((\pi 1)^{n_{r-1}} \cdots (\pi r)^{n_r}\) has a non-primitive antecedent by the Burrows-Wheeler transform, then the \( n_i \) have a common factor \( k \). There exist (see below) non-minimal discrete interval exchange transformations which do not satisfy that condition, and thus words such as \( 32221 \) which have no antecedent at all by the Burrows-Wheeler transformation.

But our Theorem I is still valid for non-primitive words: the proof in the first direction does not use the primitivity, while in the reverse direction we write \( w = u^k \), apply our proof to the primitive \( u \), and check that \( u^{2k} \) occurs also in a trajectory.

**Two permutations.** An extension of Theorem I which fails is to consider, as the dynamicians do [13], interval exchange transformations defined by permutations \( \pi \) and \( \pi' \); this amounts to coding the interval \( \Delta_i \) by \( \pi' i \) instead of \( i \). A simple counter-example will be clearer than a long definition:
take points $x_1, \ldots, x_9$ labelled 223331111 and send them to 111133322 by a (minimal) discrete 3-interval exchange transformation, but where the points are not labelled as in Definition 3 (namely $T x_1 = x_8, T x_3 = x_5$ etc...). Then $w = 123131312$ is such that $ww$ occurs in trajectories of $T$ but $B(w) = 323311112$.

3. Building clustering words

Theorem [11] provides two different ways to build clustering words, from infinite trajectories either of discrete (or rational) interval exchange transformations or of continuous aperiodic interval exchange transformations. For $r = 2$ and the permutation $\pi 1 = 2, \pi 2 = 1$, the first ones give all the periodic balanced words, and the second ones gives (by Proposition 5 below) all infinite Sturmian words; both these ways of building clustering words on two letters are used, explicitly or implicitly, in [8].

The use of discrete interval exchange transformations leads naturally to the question of characterizing all minimal discrete $r$-interval exchange transformations through their length vector; this has been solved by [10] for $n = 3$ and $\pi 1 = 3, \pi 2 = 2, \pi 3 = 1$: if the length vector is $(n_1, n_2, n_3)$, minimality is equivalent to $(n_1 + n_2)$ and $(n_2 + n_3)$ being coprime. Thus

Example 1. The discrete interval exchange 111122333 → 333221111, gives rise to the perfectly clustering word 122131313.

The same reasoning extends to other permutations: for $\pi 1 = 2, \pi 2 = 3, \pi 3 = 1$, minimality is equivalent to $n_1$ and $(n_2 + n_3)$ being coprime; for $\pi 1 = 3, \pi 2 = 1, \pi 3 = 2$, minimality is equivalent to $n_3$ and $(n_2 + n_1)$ being coprime; for other permutation on these three letters, $T$ is never minimal.

For $r \geq 4$ intervals, the question is still open. An immediate equivalent condition for non-minimality is $\sum_{i=1}^{m} s_{w_i} = 0$ for $m < n_1 + \cdots + n_r$ and $w_1 \cdots w_m$ a word occurring in a trajectory. It is easy to build non-minimal examples satisfying such an equality for simple words $w$, for example for $r = 4$ and $\pi 1 = 4, \pi 2 = 3, \pi 3 = 2, \pi 4 = 1$, $n_1 = n_2 = n_3 = 1$ gives non-minimal examples for any value of $n_4$, the equality being satisfied for $w = 24^q$ if $n_4 = 3q$, $w = 14^{q+1}$ if $n_4 = 3q + 1$, $w = 34^q$ if $n_4 = 3q + 2$. Similarly, the following example shows how we still do get clustering words, but they may be somewhat trivial.

Example 2. The discrete interval exchange 111233444 → 444332111 satisfies the above equality for $w = 14$; it is non-minimal and gives two perfectly clustering words on smaller alphabets, 41 and 323.

To study continuous aperiodic interval exchange transformations we need a technical condition called i.d.o.c. [9] which states that the orbits of the discontinuities of $T$ are infinite and disjoint. It is proved in [9] or in [13] that this condition implies aperiodicity and minimality, and that, if $\pi$ is primitive, i.e. $\pi \{1, \ldots, d\} \neq \{1, \ldots, d\}$ for $d < r$, then the $r$-interval exchange transformation with probability vector $(\alpha_1, \ldots, \alpha_r)$ and permutation $\pi$ satisfies the i.d.o.c. condition if $\alpha_1, \ldots, \alpha_r$ and 1 are rationally independent. We can now prove

Proposition 5. Let $w = w_1 \cdots w_n$ be a primitive word on $A = \{1, \ldots, r\}$, such that every letter of $A$ occurs in $w$. Then $w$ is $\pi$-clustering if and only if $ww$ occurs in a trajectory of a continuous $r$-interval exchange transformation with permutation $\pi$, satisfying the i.d.o.c. condition.

Proof. The “if” direction is as in Theorem [11]. To get the “only if”, we generate $w$ by a minimal discrete interval exchange transformation as in (2) of Theorem [11] and thus $\pi$ is primitive. Then
we replace it by a continuous periodic interval exchange transformation as in the proof that (3) implies (4). But, because cylinders are always semi-open intervals, if a given word $ww$ occurs in a trajectory of a continuous $r$-interval exchange transformation with permutation $\pi$ and probability vector $(\alpha_1, \ldots, \alpha_r)$, it occurs also in trajectories of every $r$-interval exchange transformation with the same permutation whose probability vector is close enough to $(\alpha_1, \ldots, \alpha_r)$. Thus we can change the $\alpha_i$ to get the irrationality condition which implies the i.d.o.c. condition.

Trajectories of interval exchange transformations satisfying the i.d.o.c. condition may be explicitly constructed via the self-dual induction algorithms of [5] for $r = 3$ and $\pi 1 = 3, \pi 2 = 2, \pi 3 = 1$, [6] for all $r$ and $\pi i = r + 1 - i$, and the forthcoming [4] in the most general case. More precisely, Proposition 4.1 of [6] shows that if the permutation is $\pi i = r + 1 - i$ (or more generally if the permutation is in the Rauzy class of $\pi i = r + 1 - i$), then there exist infinitely many words $ww$ in the trajectories. It also gives a sufficient condition for building such words: if a bispecial word $w$, a suffix $s$ and a prefix $p$ of $w$ are such that $pw = ws$, then both $pp$ and $ss$ occur in the trajectories. In turn, a recipe to achieve that relation is given in (i) of Theorem 2.8 of [6]: we just need that in the underlying algorithm described in Section 2.6 of [6], either $p_n(i) = i$ or $m_n(i) = i$ (except for some initial values of $n$, where, for $i = 1$, $p$ and $s$ are longer than $w$). Many explicit examples of $ww$ have been built in this way.

- For $r = 3$ in [5], $w = A_k$, $w = B_k$ in Proposition 2.10,
  Example 3. 1313131222 and 1221312213121313 are perfectly clustering.
- For $r = 4$ in [7], $w = M_2(k)$, $w = P_3(k)M_1(k)$ in Lemma 4.1 and in Lemma 5.1,
  Example 4. $2^m(3141)^n32$ are perfectly clustering for any $m \geq 3$ and $n \geq 2$.
- For all $r = n$ in [8], $w = P_{k,1,1}$, $w = P_{k,n-i+1,n-i+1,1}$, $w = M_{k,n+1-i,1,n+1-i}$ in Theorem 12;
  Example 5. 52524342525161525161525161525161 is perfectly clustering.

For other permutations, we shall describe in [4] an algorithm generalizing the one in [6]. We also construct an example of an interval exchange transformation which does not produce infinitely many $ww$. For the permutation $\pi 1 = 4, \pi 2 = 3, \pi 3 = 1, \pi 4 = 2$, examples can be found in Theorem 5.2 of [6], with $w = P_{1, q_n}M_{2, q_n}$, $w = P_{2, q_n}M_{3, q_n}$, $w = P_{3, q_n}M_{1, q_n}$,

Example 6. 4123231312412 is $\pi$-clustering.

We remark that our self-dual induction algorithms for aperiodic interval exchange transformations generate families of nested clustering words with increasing length, and thus may be more efficient in producing very long clustering words than the more immediate algorithm using discrete interval exchange transformations.

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**INSTITUT DE MATHÉMATIQUES DE LUMINY, CNRS - FRE 3529, CASE 907, 163 AV. DE LUMINY, F13288 MARSEILLE CEDEX 9, FRANCE AND FÉDÉRATION DE RECHERCHE DES UNITÉS DE MATHÉMATIQUES DE MARSEILLE, CNRS - FR 2291**

E-mail address: ferenczi@iml.univ-mrs.fr

**INSTITUT CAMILLE JORDAN, UNIVERSITÉ CLAUDE BERNARD LYON 1, 43 BOULEVARD DU 11 NOVEMBRE 1918, F69622 VILLEURBANNE CEDEX, FRANCE AND DEPARTMENT OF MATHEMATICS AND TURKU CENTRE FOR COMPUTER SCIENCE, UNIVERSITY OF TURKU, 20014 TURKU, FINLAND.**

E-mail address: zamboni@math.univ-lyon1.fr