On $k$-Maximal Submonoids, with Applications in Combinatorics on Words

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Abstract
We define the notion of a $k$-maximal submonoid of the free monoid $A^*$, where $A$ is a finite alphabet. A submonoid $M$ is $k$-maximal if there does not exist another submonoid generated by at most $k$ words containing $M$. We prove that the intersection of two 2-maximal submonoids is either the empty word or a submonoid generated by one primitive word. As a consequence, for every submonoid $M$ generated by two words that do not commute, there exists a unique 2-maximal submonoid containing $M$. We aim to show that this algebraic framework can be used to introduce a novel approach in combinatorics on words. Indeed, the notion of a primitive word can be interpreted in our framework by saying that this word generates a 1-maximal submonoid. Following this analogy, we call primitive pairs those pairs of nonempty words that generate a 2-maximal submonoid. Primitive pairs therefore represent an algebraic generalization of the classical notion of a primitive word. As an immediate consequence of our results, we have that for every pair of nonempty words $\{x, y\}$ such that $xy \neq yx$ there exists a unique primitive pair $\{u, v\}$ such that $x$ and $y$ can be written as concatenations of copies of $u$ and $v$. We call the pair $\{u, v\}$ the binary root of the pair $\{x, y\}$, in analogy with the classical notion of root of a single word. For a single word $w$, we say that $\{x, y\}$ is a binary root of $w$ if $w$ can be written as a concatenation of copies of $x$ and $y$ and $\{x, y\}$ is a primitive pair. The binary root of a single word is not, in general, unique. However, we prove that every word $w$ has at most one binary root $\{x, y\}$ such that $|x| + |y| < \sqrt{|w|}$. That is, the binary root of a word is unique provided the length of the word is sufficiently large with respect to the size of the root.

Our results can also be compared to previous approaches that investigate pseudo-repetitions, where a morphic or an antimorphic involutive function $\theta$ is defined on $A^*$. A word $w$ is called a $\theta$-power if there exists a word $v$ such that $w$ can be factored using copies of $v$ and $\theta(v)$ — otherwise the word $w$ is called $\theta$-primitive. If $v$ is a $\theta$-primitive word, then it is called the $\theta$-primitive root of $w$. Of course, since the same applies to the word $\theta(w)$, these definitions can be given in terms of the pair $\{w, \theta(w)\}$ and considering as the root the pair $\{v, \theta(v)\}$. With our approach, we fully generalize this setting by considering as a root any pair of words $\{x, y\}$, i.e., dropping the relation between the components of the pair.

Finally, we discuss the case of infinite words, where the notion of a binary root represents a new refinement in the classical dichotomy periodic/aperiodic.
1 Introduction

The structure of submonoids of the free monoid is a classical subject in formal language theory. Every subset $X$ of the free monoid $A^*$ over a finite alphabet $A$ generates a submonoid $X^*$ under the operation of concatenation of words. For every submonoid $M$ of the free monoid $A^*$, there exists a unique set of words $X$ that generates $M$ and is minimal for inclusion. In fact, $X$ is the set of nonempty words of $M$ that cannot be written as a product of two nonempty words of $M$. The submonoid $M$ is free if every word of $M$ can be expressed as a product of elements of $X$ in a unique way, and in this case the basis $X$ generating $M$ is a code. A fundamental result in the theory of codes is the so-called Defect Theorem, which states that for every finite nonempty set $X$ of $A^*$, the basis $Y$ generating the minimal (w.r.t. inclusion) free submonoid containing $X$ is either equal to $X$, if $X$ is a code, or verifies $|Y| \leq |X| - 1$. The cardinality of such a set $Y$ is called the free rank of $X$.

If one considers maximality instead of minimality, it is obvious that the maximal (always w.r.t. inclusion) submonoid containing a subset $X$ of $A^*$ is $A^*$ itself. The problem is no more trivial if one relativizes the notion of maximality to the number of generators of the maximal submonoid. The novelty of our approach indeed consists in fixing an integer $k$ and asking for a maximal submonoid generated by at most $k$ elements containing $X$. Such a submonoid may not exist (for example if $k = 1$ and $X$ is equal to $\{ab, ba\}$) or, if it exists, may not be unique. Following this idea, we say that a submonoid $M$ of $A^*$ is $k$-maximal if there does not exist another submonoid generated by at most $k$ words containing $M$. For example, over $A = \{a, b, c\}$, we have that $\{a, bc\}$ is 2-maximal, whereas $\{a, aba\}$ is not, since it is contained in $\{a, bc\}$. Of course, for every $k \geq |A|$, the only $k$-maximal submonoid of $A^*$ is $A^*$ itself.

We are specially interested in the case $k = 2$. It is known (cf. [11]) that the intersection of two submonoids generated by two elements is a submonoid that is generated either by at most 2 words or by an infinite number of words. We prove in Theorem 12 that the intersection of two 2-maximal submonoids is either the empty word or a submonoid generated by one primitive word. As a consequence, for every submonoid $M$ generated by two words that do not commute, there exists a unique 2-maximal submonoid containing $M$. Moreover, known results in combinatorics on words show that the intersection of two 1-maximal submonoids consists of the empty word only, that is, a submonoid generated by 0 elements. Therefore, it is natural to ask whether, for every $k > 0$, the intersection of two $k$-maximal submonoids is generated by at most $k - 1$ elements. We answer negatively to this question, by showing an example of two 7-maximal submonoids whose intersection cannot be generated by less than 7 elements. We leave open the question do determine whether the intersection of two 2-maximal submonoids is always generated by less than $k$ elements for $2 < k < 7$.

Theorem 12 is the basis of the theory developed in the rest of the paper, where we show that our findings can be used to describe a new kind of hidden structure in finite and infinite words.

Indeed, the definition of $k$-maximal submonoid has an immediate simple connection with the area of combinatorics on words, as if $v$ is a nonempty word, then the submonoid $\{v\}$ is 1-maximal if and only if the word $v$ is primitive. We think that those pairs of nonempty words that generate a 2-maximal submonoid, that we call primitive pairs, are of particular interest in combinatorics on words, as they represent an algebraic generalization of the classical notion of primitive word. Some important properties of primitive words can be extended to primitive pairs. For example, it is well known that a primitive word $x$ does not have internal occurrences in $x^2$. We show that if $\{x, y\}$ is a primitive pair, then neither $xy$ nor $yx$ occurs internally in a word of $\{x, y\}^3$.

As a consequence of Theorem 12, we have that for every pair of nonempty words $\{x, y\}$ such that $xy \neq yx$ there exists a unique primitive pair $\{u, v\}$ such that $x$ and $y$ can be written as concatenations of copies of $u$ and $v$. We call the pair $\{u, v\}$ the binary root of the pair $\{x, y\}$, in analogy with the classical notion of root of a single word. For a single word $w$, we say that $\{x, y\}$
is a binary root of \( w \) if \( w \) can be written as a concatenation of copies of \( x \) and \( y \) and \( \{ x, y \} \) is a primitive pair. The binary root of a single word is not, in general, unique. However, we prove that every primitive word \( w \) has at most one binary root \( \{ x, y \} \) such that \(|x| + |y| < \sqrt{|w|}\). That is, the binary root of a primitive word is unique provided the length of the word is sufficiently large with respect to the size of the root. Another question we leave open is that of determining a tight bound on the length of the word that provides the uniqueness of the binary root.

Our results can also be compared to previous approaches that investigate pseudo-repetitions, as considered by Gawrychowski, Manea and Nowotka \cite{GawrychowskiMN15} and by Gawrychowski et al. \cite{GawrychowskiMN16}, where a morphic or an antimorphic involutive function \( \theta \) is defined on the set of words \( A^* \)—this idea stems from the seminal paper of Czeizler, Kari and Seki \cite{CzeizlerKS98}, where originally \( \theta \) was the Watson-Crick complementarity function and the motivation was the discovery of hidden repetitive structures in biological sequences. A word \( w \) is called a \( \theta \)-power if there exists a word \( v \) such that \( w \) can be factored using copies of \( v \) and \( \theta(v) \)—otherwise the word \( w \) is called \( \theta \)-primitive. If \( v \) is a \( \theta \)-primitive word, then it is called the \( \theta \)-primitive root of \( w \). Of course, since the same applies to the word \( \theta(w) \), these definitions can be given in terms of the pair \( \{ w, \theta(w) \} \) and considering as the root the pair \( \{ v, \theta(v) \} \). With our results, we fully generalize this setting by considering as a root any pair of words \( \{ x, y \} \), i.e., dropping the relation between the components of the pair.

In the context of infinite words, we extend our Theorem \( \ref{thm:main} \) and prove that if \( w \) is an infinite aperiodic word, then there exists at most one primitive pair \( \{ x, y \} \) such that \( w \) can be written as a concatenation of copies of \( x \) and \( y \). The notion we introduce in this paper therefore represents a refinement in the classical dichotomy periodic/aperiodic for infinite words, as there exist words that have a sort of bi-period. We think that this notion can be exploited to detect a new kind of hidden repetitive structure in words.

\section{Preliminaries}

Given a finite nonempty set \( A \), called the alphabet, with \( A^* \) (resp. \( A^* \setminus \{ \varepsilon \} \)) we denote the free monoid (resp. free semigroup) generated by \( A \), i.e., the set of all finite words (resp. all finite nonempty words) over \( A \).

The length \(|w|\) of a word \( w \in A^* \) is the number of its symbols. The length of the empty word \( \varepsilon \) is 0. For a word \( w = uvz \), with \( u, v, z \in A^* \), we say that \( v \) is a factor of \( w \). Such a factor is called internal if \( u, z \neq \varepsilon \), a prefix if \( u = \varepsilon \), or a suffix if \( z = \varepsilon \). A word \( w \) is primitive if \( w = v^n \) implies \( n = 1 \), otherwise it is called a power. Equivalently, \( w \) is primitive if and only if it does not occur internally (i.e., if it occurs, then it is a prefix or a suffix) in \( w^2 \).

As it is well known, given two words \( x, y \), one has \( xy = yx \) if and only if \( x \) and \( y \) are powers of the same word, i.e., there exists a word \( z \) such that \( x = z^n \) and \( y = z^m \), for some integers \( n, m \).

We let \( A^w \) denote the set of infinite words over \( A \), that are infinite concatenations of symbols from \( A \). An infinite word over \( A \) is called ultimately periodic when there exist \( u, v \in A^* \) such that \( w = uvv \cdots \). When \( u = \varepsilon, w \) is called (purely) periodic. A word that is not ultimately periodic is called aperiodic.

Given a subset \( X \) of \( A^* \), we denote by \( X^* \) the submonoid of \( A^* \) generated by \( X \) (under concatenation). Conversely, given a submonoid \( M \) of \( A^* \), there exists a unique set \( X \) that generates \( M \) and is minimal for set inclusion. In fact, \( X \) is the set

\[ X = (M \setminus \{ \varepsilon \}) \setminus ((M \setminus \{ \varepsilon \})^2), \]

i.e., \( X \) is the set of nonempty words of \( M \) that cannot be written as a product of two nonempty words of \( M \). The set \( X \) will be referred to as the minimal generating set of \( M \), or the set of generators of \( M \).
Let $M$ be a submonoid of $A^*$ and $X$ its minimal generating set. $M$ is said to be free if any word of $M$ can be uniquely expressed as a product of elements of $X$. The minimal generating set of a free submonoid $M$ of $A^*$ is called a code; it is referred to as the basis of $M$. It is easy to see that a set $X$ is a code if and only if, for every $x, y \in X$, $x \neq y$, one has $xX^* \cap yX^* = \emptyset$. We say that $X$ is a prefix code (resp. a suffix code) if for all $x, y \in X$, one has $x \cap yA^* = \emptyset$ (resp. $x \cap A^*y = \emptyset$). A code is a bifix code if it is both a prefix and a suffix code. It follows from elementary automata theory that if $X$ is a prefix code, then there exists a DFA $A_X$ recognizing $X^*$ whose set of states $Q_X$ verifies (cf. [2]):

$$|Q_X| \leq \sum_{x \in X} |x| - |X| + 1.$$  

A submonoid $M$ of $A^*$ is called pure (cf. [19]) if for all $w \in A^*$ and $n \geq 1$,

$$w^n \in M \Rightarrow w \in M.$$  

By Tilson’s result [20] one has that any nonempty intersection of free submonoids of $A^*$ is free. As a consequence, for any subset $X \subseteq A^*$, there exists the smallest free submonoid containing $X$.

Here we mention the well-known Defect Theorem (cf. [1], [15, Chap. 1], [16, Chap. 6]), a fundamental result in the theory of codes that provides a relation between a given subset $X$ of $A^*$ and the basis of the minimal free submonoid containing $X$ (called the free hull of $X$).

**Theorem 1 (Defect Theorem).** Let $X$ be a finite nonempty subset of $A^*$. Let $Y$ be the basis of the free hull of $X$. Then either $X$ is a code, and $Y = X$, or

$$|Y| \leq |X| - 1.$$  

As in [10], given a set $X \subseteq A^*$, we let $r_f(X)$ denote the cardinality of the basis of the free hull of $X$, called the free rank of $X$. Notice that for any subset $X \subseteq A^*$, $X$ and $X^*$ have the same free rank. Furthermore, by $r_c(X)$ we denote the combinatorial rank of $X$, defined by:

$$r_c(X) = \min\{|Y| \mid Y \subseteq A^*, X \subseteq Y^*\}.$$  

With this notation, the Defect Theorem can be stated as follows.

**Theorem 2.** Let $X$ be a finite nonempty subset of $A^*$. Then $r_f(X) \leq |X|$, and the equality holds if and only if $X$ is a code.

Note that, for any $X \subseteq A^+$, one has

$$r_c(X) \leq r_f(X) \leq |X|.$$  

**Example 3.** Let $X = \{aa, ba, baa\}$. One can prove that $X$ is a code, hence we have $r_f(X) = 3$, while $r_c(X) = 2$ since $X \subset \{a, b\}^*$. For $X = \{aa, aaa\}$, we have $r_c(X) = r_f(X) = 1$.

The dependency graph (cf. [10]) of a finite set $X \subset A^*$ is the graph $G_X = (X, E_X)$ where $E_X = \{(u, v) \in X \times X \mid uX^* \cap vX^* \neq \emptyset\}$. Note that if $X$ is a code, then $G_X$ has no edge. In [9] and [10], the following useful lemma is proved.

**Lemma 4 (Graph Lemma).** Let $X \subseteq A^*$ be a finite set that is not a code. Then

$$r_f(X) \leq c(X) < |X|,$$

where $c(X)$ is the number of connected components of $G_X$.

**Example 5.** Let $X = \{a, ab, abc, bca, cab\}$. We have $acba = a \cdot cba = acb \cdot a$ and $abca = a \cdot bca = abc \cdot a$. The basis of the free hull of $X$ is $Y = \{a, ab, bc, cb\}$, hence $r_f(X) = 4$. Furthermore, $r_c(X) = 3$ and $c(X) = 4$, as shown in Figure [1].

**Remark.** If $X \subseteq A^*$ is a set of cardinality 2, then it is easy to see that $r_c(X) = r_f(X)$.  

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Figure 1 The dependency graph of $X = \{a, ab, abc, bca, acb, cba\}$.

3 $k$-maximal Monoids

With $\mathcal{M}_k$ we denote the family of submonoids of $A^*$ having at most $k$ generators in $A^+$. The following definition is fundamental for the theory developed in this paper.

Definition 6. A submonoid $M \in \mathcal{M}_k$ is $k$-maximal if for every $M' \in \mathcal{M}_k$, $M \subseteq M'$ implies $M = M'$.

In other words, $M$ is $k$-maximal if it is not possible to find another submonoid generated by at most $k$ words containing $M$.

Example 7. Let $A = \{a, b, c\}$. The submonoid $M = \{a, abca\}^*$ is not 2-maximal since it is contained in $\{a, bc\}^*$. On the contrary, $\{a, bc\}^*$ is 2-maximal.

Example 8. Let $A = \{a, b, c, d\}$. The submonoid $\{a, cb, dcb\}^*$ is 3-maximal, whereas $\{a, cb, dcdb\}^*$ is not 3-maximal since it is contained in $\{a, d, cb\}^*$.

Remark. For every word $v \in A^+$, the submonoid $\{v\}^*$ (denoted simply by $v^*$ in the rest of the paper) is 1-maximal if and only if $v$ is a primitive word. Moreover, if $|X| = |A| = k$, then $X^*$ is $k$-maximal if and only if $X = A$.

We have the following property.

Proposition 9. Let $M$ be a $k$-maximal submonoid and $X$ its minimal generating set. Then, $X$ is a bifix code.

Proof. By contradiction, if $X$ is not prefix (resp. not suffix) then there exist $u, v \in X$ and $t \in A^+$ such that $v = ut$ (resp $v = tu$). It follows that $X^* \subseteq (X \setminus \{v\} \cup \{t\})^*$, whence $X^* = M$ is not $k$-maximal.

Remark. By Proposition 7, it follows that if $X^*$ is $k$-maximal, then $r_f(X) = r_f(X) = k$. The inverse implication does not hold in general. For example, the submonoid $X^* = \{a, cb, dcdb\}^*$ of Example 8 has free and combinatorial rank both equal to 3 but is not 3-maximal.

Proposition 10. Let $M$ be a $k$-maximal submonoid. Then $M$ is a pure submonoid.

Proof. We have to show that, for every $z \in A^*$, if $z^n \in M$, for some $n \geq 1$, then $z \in M$. Let $X$ be the minimal generating set of $M$. If $z^n \in M$, for some $n > 1$, then the set $X \cup \{z\}$ is not a code. By the Defect Theorem (Theorem 3), there exist $u_1, u_2, \ldots, u_k \in A^*$ such that $(X \cup \{z\})^* \subseteq \{u_1, u_2, \ldots, u_k\}^*$. Since $X^* \subseteq \{u_1, u_2, \ldots, u_k\}^*$ and $X^*$ is $k$-maximal, we have that $X = \{u_1, u_2, \ldots, u_k\}$. Therefore, $X \cup \{z\} \subseteq X^*$, hence $z \in X^*$.

As a direct consequence of Proposition 10 we have that a $k$-maximal submonoid is generated by primitive words. However, note that not any set of $k$ primitive words generates a $k$-maximal monoid (e.g., $X = \{ab, ba\}^*$ is not 2-maximal).

Of special interest for our purposes are the submonoids generated by two words. They have been extensively studied in literature (cf. [14, 11, 18, 13]) and play an important role in some fundamental aspects of combinatorics on words.
The reader may observe that, as a consequence of some well-known results in combinatorics on words, the submonoids in \( M_1 \) have the following important property: If \( x^* \) and \( u^* \) are 1-maximal submonoids (i.e., \( x \) and \( u \) are primitive words) then \( x^* \cap u^* = \{ \varepsilon \} \). Next Theorem 12 which represents the main result of this section, can be seen as a generalization of this result to the case of 2-maximal submonoids.

It is known (see [11]) that if \( X \) and \( U \) have free rank 2, then the intersection \( X^* \cap U^* \) is a free monoid generated either by at most two words or by an infinite set of words.

**Example 11.** Let \( X_1 = \{ abca, be \} \) and \( U_1 = \{ a, bcbe \} \). One can verify that \( X_1^* \cap U_1^* = \{ abca, beca \}^* \). Let \( X_2 = \{ aab, aba \} \) and \( U_2 = \{ a, baab \} \). Then \( X_2^* \cap U_2^* = \{ a(ababa)^*baab \}^* \).

In the previous example, we have two submonoids that are not 2-maximal. Indeed, \( X_1^*, U_1^* \subseteq \{ a, be \}^* \) and \( X_2^*, U_2^* \subseteq \{ a, b \}^* \). We now address the question of finding the generators of the intersection of two 2-maximal submonoids. The following theorem is the starting point of our investigation on binary roots, that we will develop in the subsequent sections.

**Theorem 12.** Let \( X = \{ x, y \} \) and \( U = \{ u, v \} \), with \( X \neq U \), be such that \( X^* \) and \( U^* \) are 2-maximal submonoids of \( A^* \). If \( X^* \cap U^* \neq \{ \varepsilon \} \), then there exists a word \( z \in A^* \) such that \( X^* \cap U^* = z^* \). Moreover, \( z \) is primitive, that is, \( X^* \cap U^* \) is 1-maximal.

**Proof.** If \( X \cap U = \{ z \} \), then trivially \( X^* \cap U^* = z^* \). If \( X \cap U = \emptyset \), let us consider the set \( Z = X \cup U \). We have that \( r_f(Z) > 2 \) since \( X^* \) and \( U^* \) are 2-maximal, and, by the Defect Theorem (Theorem 11), \( r_f(Z) < 4 \) since \( Z \) is not free (as \( X^* \cap U^* \) contains a nonempty word).

Hence, the rank of \( Z \) is equal to 3.

Let \( z \) be a generator of \( X^* \cap U^* \). So, \( z = x_1x_2 \cdots x_m = u_1u_2 \cdots u_n \), with \( m, n \geq 1 \), \( x_i \in X \) and \( u_j \in U \). Clearly, since \( z \) is a generator, for every \( p < m \) and \( q < n \) one has \( x_1x_2 \cdots x_p \neq u_1u_2 \cdots u_q \). Moreover, we can suppose, without loss of generality, that \( x_1 = x \) and \( u_1 = u \). We want to prove that \( z \) is the unique generator of \( X^* \cap U^* \). By contradiction, suppose that there exists another generator \( z' \neq z \) of \( X^* \cap U^* \), and let \( z' = x_1'x_2' \cdots x_r' = u_1'u_2' \cdots u_r' \). If \( x_1' \neq x_1 \), then \( x_1' = y \) and we have \( xZ^* \cap uZ^* \neq \emptyset \) and \( yZ^* \cap u_1'Z^* \neq \emptyset \). In both cases \((u_1' = u \text{ or } u_1' = v)\), we have that the graph \( G_z \) has two edges, i.e., \( c(Z) = 2 \), which is impossible by the Graph Lemma. So \( x_1 = x_1' = x \). In the same way we prove that \( u_1 = u_1' = u \), and therefore in the graph \( G_z \) there is only one edge, namely the one joining \( x \) and \( u \).

\[
\begin{array}{ccc}
x & & y \\
  \downarrow & & \downarrow \\
u & & v
\end{array}
\]

Let \( h = \max\{ i \mid x_j = x_j' \forall j \leq i \} \) and \( k = \max\{ i \mid u_j = u_j' \forall j \leq i \} \). The hypothesis that \( z \neq z' \) implies that \( h < m \) and \( k < n \). We show that this leads to a contradiction, and then we conclude that \( z = z' \) is the unique generator of \( X^* \cap U^* \).

Without loss of generality, we can suppose that \( x_1x_2 \cdots x_h \) is a prefix of \( u_1u_2 \cdots u_k \). Hence, there exists a nonempty word \( t \) such that \( x_1x_2 \cdots x_ht = u_1u_2 \cdots u_k \). By definition of \( h \), \( x_{h+1} \neq x_{h+1}' \), and we can suppose that \( x_{h+1} = x \) and \( x_{h+1}' = y \). Then,
\[
\begin{align*}
tu_{k+1} \cdots u_n & = x_{h+1} \cdots x_m = x \cdots x_m \\
tu_{k+1}' \cdots u_n' & = x_{h+1}' \cdots x_r' = y \cdots x_r'.
\end{align*}
\]

Set \( Z_1 = X \cup U \cup \{ t \} \). We have
\[
\begin{align*}
tZ_1^* \cap xZ_1^* & \neq \emptyset \\
tZ_1^* \cap yZ_1^* & \neq \emptyset.
\end{align*}
\]

Thus, the graph \( G_{Z_1} \) contains the edges depicted in figure:
By the Graph Lemma, then, the free rank of $Z_t$ is at most 2, and this contradicts the 2-maximality of $X^*$ and $U^*$.

Finally, let us prove that $z$ is primitive. Since $X^*$ and $Y^*$ are 2-maximal, by Proposition [10], they are both pure, hence also their intersection $z^*$ is pure. But it is immediate that $z^*$ is pure if and only if $z$ is primitive.

▶ Corollary 13. Let $M$ be a submonoid of $A^*$ generated by two words $x$ and $y$ such that $xy \neq yx$. Then, there exists a unique 2-maximal submonoid containing $M$.

We have shown that the intersection of two 2-maximal submonoids is generated by at most one element. Moreover, we know that the intersection of two 1-maximal submonoids is the empty word, i.e., it is generated by zero elements. Thus, it is natural to ask if in general, for every $k \geq 1$, the intersection of two $k$-maximal submonoids is generated by at most $k - 1$ elements. The following example provides a negative answer to this question.

▶ Example 14. Let $X = \{ab, bc, bd, cf, ga, dt, sa\}$ and $U = \{abc, abd, ts, f, gad, dtb, csa\}$. Both $X^*$ and $U^*$ are 7-maximal submonoids of $\{a, b, c, d, f, s, t\}^*$. One can verify that the basis of $X^* \setminus U^*$ has cardinality 7 and is

$$\{abcgabc, abcgabd, abdtsabc, abdtsabd, gadtsabc, gadtsabd, dtbcsa\}.$$  

▶ Open Problem 1. For $k$ such that $2 < k < 7$, is the intersection of two $k$-maximal submonoids always either the empty word or a submonoid generated by $h$ elements, with $h < k$? And, if so, is this intersection $h$-maximal?

For an upper bound on the length of the word that generates the intersection of two 2-maximal submonoids, we have the following proposition.

▶ Proposition 15. With the hypotheses of Theorem [12]

$$|z| < (|x| + |y|)(|u| + |v|).$$  

Proof. Let $A_X$ (resp. $A_U$) be a DFA recognizing $X^*$ (resp. $U^*$) and $Q_X$ (resp. $Q_Y$) its set of states. Since $X$ and $U$ are bifix codes, we have $|Q_X| < |x| + |y|$ and $|Q_U| < |u| + |v|$. Then the automaton $A$ recognizing $X^* \cap U^*$ has a set of states $Q$ such that $|Q| < (|x| + |y|)(|u| + |v|)$. By Theorem [12], $A$ is composed by only one cycle, labeled by $z$. Thus, $|z| < (|x| + |y|)(|u| + |v|)$.

▶ Open Problem 2. Find a tight bound on the length of $z$ in terms of the lengths of $x$ and $y$.

4 Some Applications in Combinatorics on Words

In the rest of this paper, we apply our algebraic framework in the context of combinatorics on words.
4.1 Primitive Pairs

We first show how the previous results can be interpreted in the terminology of combinatorics on words. Let us start with the remark that a word $x \in A^+$ is primitive if and only if

$$x \in u^*, u \in A^+ \Rightarrow x = u.$$  

With our definition of maximality, we have that a word $x \in A^+$ is primitive if and only if the monoid $x^*$ is $1$-maximal. Inspired by this observation, we give the following definition.

**Definition 16.** A pair $\{x, y\}$ of nonempty words over $A^+$ is a primitive pair if

$$\{x, y\} \subset \{u, v\}^*, u, v \in A^+ \Rightarrow \{x, y\} = \{u, v\}.$$  

Therefore, coherently with the definition of a primitive word, we can say that a pair $\{x, y\}$ of words in $A^+$ is a primitive pair if and only if the submonoid $\{x, y\}^*$ is $2$-maximal.

Analogously to the case of a single word, a pair $\{x, y\}$ that is not a primitive pair can in general be written in several ways as a concatenation of copies of two other words.

**Example 17.** The words $abca$ and $bc$ are primitive words, yet the pair $\{abca, bc\}$ is not a primitive pair, since $\{abca, bc\}^* \subseteq \{a, bc\}^*$, hence $\{abca, bc\}^*$ is not $2$-maximal. The pair $\{abcabc, bcabca\}$ can be written as concatenations of copies of both $\{abca, bc\}$ and $\{a, bcabc\}$.

However, as a restatement of Corollary 13 in terms of primitive pairs, we have the following result.

**Theorem 18.** Let $\{x, y\}$ be a pair of nonempty words such that $xy \neq yx$. Then, there exists a unique primitive pair $\{u, v\}$, called the binary root of $\{x, y\}$, such that $x$ and $y$ can be written as concatenations of copies of $u$ and $v$.

**Example 19 (Example 17 continued).** There exists a unique way to decompose each word of the pair $\{abcabc, bcabca\}$ as a concatenation of words of a primitive pair, and this pair is $\{a, bc\}$.

As it is well known, a primitive word $x$ does not have internal occurrences in $xx$. We are now showing that if $\{x, y\}$ is a primitive pair, then neither $xy$ nor $yx$ occurs internally in a word of $\{x, y\}^3$.

**Theorem 20.** Let $\{x, y\}$ be a primitive pair. Then neither $xy$ nor $yx$ occurs internally in a word of $\{x, y\}^3$.

The proof is technical and is reported to the appendix due to space constraints.

**Example 21.** Let $x = abcabc$, $y = beaabcabc$. Then $xy$ has an internal occurrence in $yxx$, yet $\{x, y\} \subset \{a, bc\}^*$. This example shows that the hypothesis that $\{x, y\}$ is a primitive pair cannot be replaced by simply requiring that $x$ and $y$ are primitive words.

4.2 Binary Root of a Single Word

In this subsection we further show how our algebraic framework can be applied to some classical notions of combinatorics on words, by introducing the concept of a binary root of a single word.

Let $w$ be a nonempty word. If $w$ is not primitive, then it can be written in a unique way as a concatenation of copies of a primitive word $r$, called the root of $w$. However, if $w$ is primitive, one can ask whether it can be written as a concatenation of copies of two words $x$ and $y$. If we further require that $\{x, y\}$ is a primitive pair, then we call $\{x, y\}$ a binary root of the word $w$. Note that the binary root of a word is not, in general, unique. For instance, for $w = abcabc$ we
have \( w = ab \cdot cbac = abeb \cdot ac \) and \( \{ab, cbac\} \) and \( \{abeb, ac\} \) are both primitive pairs, i.e., they are both binary roots of \( w \). However, if we search for a sort of “high repetitiveness” (that is, we additionally require that the size \( |x| + |y| \) of the binary root \( \{x, y\} \) is “short” with respect to the length of \( w \) then we obtain again the uniqueness. This is shown in the next theorem.

**Theorem 22.** Let \( w \) be a primitive word. Then \( w \) has at most one binary root \( \{x, y\} \) such that \( |x| + |y| < \sqrt{|w|} \).

**Proof.** Suppose by contradiction there exists another binary root \( \{u, v\} \) of \( w \) with \(|u| + |v| < \sqrt{|w|} \).

Take \( X = \{x, y\} \) and \( U = \{u, v\} \). By Theorem 12 there exists a primitive word \( z \) and an integer \( n \) such that \( w = z^n \). As \( w \) is primitive, \( w = z \) and \( n = 1 \). By Proposition 15 we have that \(|w| < (|x| + |y|)(|u| + |v|) < \sqrt{|w|} \cdot \sqrt{|w|} = |w| \), a contradiction. □

The following example shows a word \( w \) that has binary roots of different sizes, but only one of size less than \( \sqrt{|w|} \).

**Example 23.** Consider the word \( w = abcaabcabc \) of length 10. The pair \( \{a, bc\} \) is the only binary root of \( w \) of size less than \( \sqrt{|w|} \).

Asking for a tight bound in the statement of Theorem 22 is of course a problem intimately related to Problem 2.

The notion of a binary root therefore reveals a hidden repetitive structure inside a word. We think that this notion can be further explored and may have applications in the area of string algorithms.

Notice that the minimal length of the binary root (intended as the sum of the lengths of the two components of the pair) is affected by the combinatorial properties of the word. For example, if \( w \) is a square-free word, then \( w \) cannot have a binary root \( \{x, y\} \) such that \(|x| + |y| < |w|/4 \), since otherwise \( w \) would contain a square \((xx, yy, xyxy \text{ or } yxyz)\).

The previous remark suggests a possible link between the notion of a binary root and the classical notion of a binary pattern, which has been deeply investigated in combinatorics on words and fully classified by J. Cassaigne [3].

### 4.3 Connections with Pseudo-primitive Words

We now show how the notion of a primitive pair can be seen as a generalization of the notion of a pseudo-primitive word (with respect to an involutive (anti-)morphism \( \theta \)) introduced in [5].

A map \( \theta : A^* \rightarrow A^* \) is a morphism (resp. antimorphism) if for each \( u, v \in A^* \), \( \theta(uv) = \theta(u)\theta(v) \) (resp. \( \theta(uv) = \theta(v)\theta(u) \)) — \( \theta \) is an involution if \( \theta(\theta(a)) = a \) for every \( a \in A \).

Let \( \theta \) be an involutive morphism or antimorphism other than the identity function. We say that a word \( w \in A^* \) is a \( \theta \)-power of \( t \) if \( w \in t\{t, \theta(t)\}^* \). A word \( w \) is \( \theta \)-primitive if there exists no nonempty word \( t \) such that \( w \) is a \( \theta \)-power of \( t \) and \(|w| > |t| \).

**Theorem 24 ([5]).** Given a word \( w \in A^* \) and an involutive (anti-)morphism \( \theta \), there exists a unique \( \theta \)-primitive word \( u \in A^* \) such that \( w = u \theta - power of \( u \). The word \( u \) is called the \( \theta \)-root of \( w \).

**Example 25.** Let \( \theta : \{a, b, c\}^* \rightarrow \{a, b, c\}^* \) the involutive morphism defined by \( \theta(a) = b \) and \( \theta(c) = c \). The \( \theta \)-root of the word \( ababab \) is \( abc \).

If \( \theta \) is an involutive morphism, we show that Theorem 23 can be obtained as a consequence of Theorem 24. If \( \theta \) is an involutive antimorphism, we obtain a slightly different formulation, from which we derive a new property of \( \theta \)-primitive words.

Given a morphism \( \theta \) and a set \( X \subseteq A^* \), \( \theta(X) \) denotes the set \( \{\theta(u) \mid u \in X\} \). We say that \( X \) is \( \theta \)-invariant if \( \theta(X) \subseteq X \).

We have the following propositions.
Proposition 26. Let \( \theta \) be an involutive (anti-)morphism and \( X \subseteq A^* \) the minimal generating set of \( X^* \). The following conditions are equivalent:

i) \( \theta(X) \subseteq X \);

ii) \( \theta(X) \subseteq X^* \);

iii) \( \theta(X) = X \).

Proof. It is sufficient to prove that i) \( \Rightarrow \) iii) and ii) \( \Rightarrow \) i).

i) \( \Rightarrow \) iii) If \( \theta(X) \subseteq X \), then \( \theta(\theta(X)) \subseteq \theta(X) \), i.e., \( X = \theta(X) \).

ii) \( \Rightarrow \) i) \( \theta(X) \subseteq X^* \) implies that, for an arbitrary \( x \in X \), \( \theta(x) = x_1x_2 \cdots x_n \), with \( x_i \in X \). It follows that \( x = \theta(\theta(x)) = \theta(x_1) \cdots \theta(x_n) \). Since \( X \) is the minimal generating set of \( X^* \), we have \( n = 1 \) and \( \theta(x_1) = x \). It follows that \( \theta(X) \subseteq X \).

Proposition 27. If \( \{x, y\} \) is \( \theta \)-invariant, then so is its root.

Proof. Let \( \{u, v\} \) be the root of \( \{x, y\} \). This means that \( \{x, y\} \subseteq \{u, v\}^* \) and \( \{u, v\}^* \) is the (unique) 2-maximal submonoid containing \( \{x, y\} \). It follows that \( \theta(\{x, y\}) \subseteq \theta(\{u, v\})^* \). Then, \( \{x, y\} = \theta(\{x, y\}) \subseteq \theta(\{u, v\})^* \). By Proposition 26 it follows that \( \theta(\{u, v\}) = \{u, v\} \).

Example 28. Let \( \theta \) be as in Example 25. The pair \( \{abcabca, abcbaca\} \) is \( \theta \)-invariant. However, it is not a primitive pair. Its binary root is the pair \( \{abc, bac\} \), which is \( \theta \)-invariant since \( \theta(abc) = bac \).

Remark. Let \( \theta \) be an involutive morphism. Then \( \{x, y\} \) is \( \theta \)-invariant if and only if \( y = \theta(x) \). If \( \theta \) is an involutive antimorphism, then \( \{x, y\} \) is \( \theta \)-invariant if and only if either \( y = \theta(x) \) or \( x = \theta(x) \) and \( y = \theta(y) \). In the last case, \( x \) and \( y \) are called \( \theta \)-palindromes.

Example 29. Let \( \theta : \{a, b, c\}^* \rightarrow \{a, b, c\}^* \) be the involutive antimorphism defined by \( \theta(a) = a \), \( \theta(b) = b \), \( \theta(c) = c \). The pair \( \{abcbaca, abcba\} \) is \( \theta \)-invariant. Its binary root is \( \{a, bcb\} \), which is \( \theta \)-invariant since composed by \( \theta \)-palindromes. With the same \( \theta \), the pair \( \{abcbabba, abbababa\} \) is \( \theta \)-invariant and its binary root is \( \{abb, bba\} \), which is \( \theta \)-invariant since \( \theta(abb) = bba \).

Proposition 30. Let \( w \in A^* \) and \( \theta \) an involutive morphism of \( A^* \). Then, \( w \) is \( \theta \)-primitive if and only if the pair \( \{w, \theta(w)\} \) is a primitive pair.

Proof. Let us suppose, by contradiction, that \( \{w, \theta(w)\} \) is a primitive pair and \( w \) is not \( \theta \)-primitive. Then there exists \( t \) such that \( w \in \{t, \theta(t)\}^* \). Hence, \( \theta(w) \in \{t, \theta(t)\}^* \), so the pair \( \{w, \theta(w)\} \) is not primitive. Conversely, let us suppose that \( w \) is \( \theta \)-primitive and \( \{w, \theta(w)\} \) is not a primitive pair. Denote by \( \{u, v\} \) its binary root. Since \( \{w, \theta(w)\} \) is \( \theta \)-invariant, then \( \{u, v\} \) is \( \theta \)-invariant, i.e., \( v = \theta(u) \). Hence, \( w \in \{u, \theta(u)\}^* \), i.e., \( w \) is not \( \theta \)-primitive.

From Theorem 18 and Proposition 30 we derive Theorem 24 when \( \theta \) is an involutive morphism.

Now, let us consider the case of antimorphisms. Reasoning analogously as we did in the proof of Proposition 30 we can prove the following result.

Proposition 31. Let \( w \in A^* \) and \( \theta \) an involutive antimorphism of \( A^* \). If the pair \( \{w, \theta(w)\} \) is a primitive pair, then \( w \) is \( \theta \)-primitive.

The converse does not hold in general, as the following example shows.

Example 32. Let \( \theta \) be the antimorphic involution of Example 29. The word \( w = abbaabbabc \) is \( \theta \)-primitive, whereas the pair \( \{w, \theta(w)\} = \{abbaabbabc, cbcabbaabba\} \) is not a primitive pair, since its binary root is the pair \( \{abba, cba\} \).

Finally, we can state the following proposition, which provides a factorization property of \( \theta \)-primitive words.
Proposition 33. Let \( w \in A^* \) and \( \theta \) an involutive antimorphism. If \( w \) is \( \theta \)-primitive and \( \{w, \theta(w)\} \) is not a primitive pair, then there exist two \( \theta \)-palindromes \( p \) and \( q \) such that \( w \in \{p, q\}^* \).

Proof. Suppose that \( \{w, \theta(w)\} \) is not a primitive pair and denote by \( \{u, v\} \) its binary root. Since \( \{w, \theta(w)\} \) is \( \theta \)-invariant, then so is \( \{u, v\} \) by Proposition 26 and \( v \not= \theta(u) \) since \( w \) is \( \theta \)-primitive. Then, \( u = \theta(u) \) and \( v = \theta(v) \) are \( \theta \)-palindromes.

Finally, we point out that our Theorem 20 can be viewed as a generalization of the following result of Kari, Masson and Seki [12]:

Theorem 34 (Theorem 12 of [12]). Let \( x \) be a nonempty \( \theta \)-primitive word. Then neither \( x \theta(x) \) nor \( \theta(x)x \) occurs internally in a word of \( \{x, \theta(x)\}^* \).

5 Infinite Words

In this section we extend our framework to the case of infinite words.

Let \( A^\omega \) denote the set of all infinite words over \( A \). For a set \( X \subseteq A^+ \), we let \( X^\omega \) denote the set of infinite concatenations of elements of \( X \), that is, \( X^\omega = \{x_1x_2x_3 \cdots \mid x_i \in X\} \). A set \( X \subseteq A^+ \) is an \( \omega \)-code if every \( w \in X^\omega \) has a unique factorization in \( X \), i.e., for all \( u, v \in X \), \( uX^\omega \cap vX^\omega = \emptyset \). An \( \omega \)-code is a code, but the converse is not, in general, true. The \( \omega \)-free hull of a set \( X \) is the smallest \( \omega \)-free finitary binoid containing \( X \) (cf. [16, Chap. 6]). Its basis is an \( \omega \)-code and the cardinality of such a basis is \( r_\omega(X) \), the \( \omega \)-rank of \( X \). A kind of defect property remains valid for infinite words:

Theorem 35. Let \( X \) be a finite nonempty subset of \( A^+ \). Let \( Y \) be the basis of the \( \omega \)-free hull of \( X \). Then either \( X \) is an \( \omega \)-code, and \( Y = X \), or
\[ |Y| \leq |X| - 1. \]

As we did in the case of submonoids, we can give an analogous definition of the dependency graph (cf. [10]) as the graph \( G_X^\omega = (X, E_X^\omega) \) where \( E_X^\omega = \{(u, v) \in X \times X \mid uX^\omega \cap vX^\omega \neq \emptyset\} \). The Graph Lemma can be then generalized as follows.

Lemma 36. Let \( X \subseteq A^+ \) a finite set that is not an \( \omega \)-code. Then
\[ r_\omega(X) \leq c_\omega(X) < |X|, \]
where \( c_\omega(X) \) is the number of connected components of \( G_X^\omega \).

Given a set \( X \subseteq A^* \), we say that \( X^\omega \) is \( \omega - k \)-maximal if, for every set \( Y \subseteq A^* \), with \( |Y| \leq k \), \( X^\omega \subseteq Y^\omega \) implies \( X = Y \). Notice that \( X^\omega \) is \( \omega - k \)-maximal if and only if \( X^* \) is \( k \)-maximal.

In fact, if \( X^* \) is \( k \)-maximal then \( X \) is a prefix code, hence it is an \( \omega \)-code.

In such a context, we have an analogous formulation of Theorem 12.

Theorem 37. Let \( X^\omega = \{x, y\}^\omega \) and \( U^\omega = \{u, v\}^\omega \), with \( X \neq U \), be \( \omega - 2 \)-maximal. If \( X^\omega \cap Y^\omega \neq \emptyset \), then there exist \( r, s \in A^* \) such that \( X^\omega \cap U^\omega = rs^\omega \). Moreover, \( r = \varepsilon \) if and only if \( X^* \cap U^* \neq \{\varepsilon\} \).

Proof. If \( X \cap U = \{z\} \), then trivially \( X^\omega \cap U^\omega = z^\omega \). If \( X \cap U = \emptyset \), let us consider the set \( Z = X \cup U \). We have that \( r_\omega(Z) > 2 \) since \( X^\omega \) and \( U^\omega \) are \( \omega - 2 \)-maximal, and, by the Defect Theorem (Theorem 33), \( r_\omega(Z) < 4 \) since \( Z \) is not an \( \omega \)-code (as \( X^\omega \cap U^\omega \) contains a nonempty word). Hence, \( r_\omega(Z) = 3 \).

Let \( z \in X^\omega \cap U^\omega \). So, \( z = x_1x_2 \cdots = u_1u_2 \cdots \), with \( x_i \in X \) and \( u_i \in U \). We can suppose, without loss of generality, that \( x_1 = x \) and \( u_1 = u \). We want to prove that \( z \) is the unique infinite...
word in $X^\omega \cap U^\omega$. By contradiction, suppose that there exists another $z' \neq z$ with $z' \in X^\omega \cap U^\omega$, and let $z' = x' \in \ldots = u' \cdot u_2 \cdots$. As in the proof of Theorem \[12] if $x' \neq x_i$ or $u'_1 \neq u_1$, then $G_Z^\omega$ has two edges, i.e., $c_{\omega}(Z) = 2$, which is impossible.

Thus, we have $x_1 = x'_1 = x$ and $u_1 = u'_1 = u$ and therefore in the graph $G_Z^\omega$ there is only one edge, precisely the one joining $x$ and $u$:

$$
\begin{array}{c}
x \\
| \\
u \\
y \\
v
\end{array}
$$

From the hypothesis that $z \neq z'$, we have that there exists an integer $h = \max\{i \mid x_j = x'_j \forall j \leq i\}$. Without loss of generality, we can suppose that $x_1 x_2 \cdots x_h$ is a prefix of $u_1 u_2 \cdots u_k$.

Hence, there exists a nonempty word $t$ such that $x_1 x_2 \cdots x_h t = u_1 u_2 \cdots u_k$.

Let us suppose that $x_{h+1} = x$ and $x'_{h+1} = y$. Then,

$t u_{k+1} \cdots = x_{h+1} \cdots = x \cdots$

$t u'_{k+1} \cdots = x'_{h+1} \cdots = y \cdots$

Set $Z_t = X \cup U \cup \{t\}$. Then,

$t Z_t^\omega \cap x Z_t^\omega \neq \emptyset$,

$t Z_t^\omega \cap y Z_t^\omega \neq \emptyset$.

So the graph $G_Z^\omega$ contains the edges depicted in figure:

By the Graph Lemma (Lemma \[36\]), the $\omega$-rank of $Z_t$ is at most 2, against the $\omega - 2$-maximality of $X^\omega$ and $U^\omega$.

Finally, let us prove that $z$ is periodic. Let $t_1, t_2, \ldots$ be the sequence of words defined as follows: For every $i \geq 1$, denoting by $j$ the smallest integer such that $u_1 u_2 \cdots u_i$ is a prefix of $x_1 x_2 \cdots x_j$, let $t_i$ be the word defined by the relation $u_1 u_2 \cdots u_i t_i = x_1 x_2 \cdots x_j$. We have that $X^* \cap U^* \neq \{\varepsilon\}$ if and only if there exists $i$ such that $t_i = \varepsilon$. In such a case, $r = \varepsilon$ and $s = u_1 u_2 \cdots u_i$. Otherwise, there exist $h, k$, with $h < k$, such that $t_h = t_k$. It follows that, for every $m \geq 0$, $u_{h+m} = u_{k+m}$. In this case, we have $z = r s^\omega$, where $r = u_1 u_2 \cdots u_h$ and $s = u_{h+1} \cdots u_k$.

\[\text{Example 38.}\] Let $X^* = \{a, bc\}^*$ and $U^* = \{ab, cb\}^*$. They are both $\omega - 2$-maximal. We have $X^* \cap U^* = \{\varepsilon\}$, while $X^\omega \cap U^\omega = ab e b c \cdots = a \cdot b c \cdot b c \cdots = a b \cdot c \cdot b c \cdots = ab (cb)^\omega$.

The following corollary is the analogous of Theorem \[22\] for infinite words.

\[\text{Corollary 39.}\] Let $w$ be an infinite aperiodic word. If there exists a primitive pair $\{x, y\}$ such that $w \in \{x, y\}^\omega$, then such a pair is unique.
So, while a purely periodic infinite word has a unique root (that is, the primitive word generating it by concatenation), there are infinite aperiodic words that are generated by a primitive pair — and in such a case this pair is unique, and can be called the binary root of the infinite word. We think that this concept may be worth further investigation, as it represents a refinement in the classical dichotomy periodic/aperiodic for infinite words.

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A Proof of Theorem 20

The following Lemma is a classical result in combinatorics on words, originally due to Lyndon and Schützenberger [17] (cf. also [15, 14, 16]).

Lemma 40. Let \( t, v \) be nonempty words such that \( tv = uv \) and \( t \neq v \). Then there exists a unique pair of words \( (p, q) \) and a unique positive integer \( m \) such that \( pq \) is primitive and

\[
t = (pq)^m, \quad v = (qp)^m, \quad u \in (pq)^\ast p.
\]

We now give the proof of Theorem 20. Let \( \{x, y\} \) be a primitive pair. Then neither \( xy \) nor \( yx \) occurs internally in a word of \( \{x, y\}^\ast \).

Proof. By symmetry, it is sufficient to prove the statement for \( xy \).

First, we claim that the word \( xy \) is primitive. Suppose by contradiction \( xy = t^n, n > 1 \). This implies that there is an occurrence of \( t \) containing the last letter of \( x \) and the first letter of \( y \). Let us write this occurrence as \( t = t_1t_2 \), where \( t_1 \) is a suffix of \( x \) and \( t_2 \) a prefix of \( y \). Then \( \{x, y\} \subset \{t_1, t_2\} \). against the primitiveness of the pair \( \{x, y\} \).

Let \( w \in \{x, y\}^3 \). The cases \( w = xxx \) and \( w = yyy \) are trivial, as \( x \) (resp. \( y \)) cannot have an internal occurrence in \( xx \) (resp. in \( yy \)) and \( \{x, y\} \) is a bifix set by Proposition 9. Let us consider the cases \( w = xyx \) and \( w = yxy \). If \( xy \) occurs internally in \( w = xyx \) (resp. in \( w = yxy \)), then so it does in \( (xy)^2 = wy \) (resp. in \( w = wv \)), in contradiction with the fact that \( xy \) is primitive.

In the cases \( w = xyx \) and \( w = yxy \), \( x \) (resp. \( y \)), would have an internal occurrence in \( xx \) (resp. \( yy \)), against the primitiveness of \( x \) (resp. of \( y \)).

The remaining cases are \( w = yxx \) and \( w = yyy \). Let us prove the case \( w = yxx \).

Let us first suppose \( |y| > |x| \). We have two subcases:

1. The internal occurrence of \( y \) does not overlap with the prefix \( y \);
2. The internal occurrence of \( y \) overlaps with the prefix \( y \).

![Figure 2](https://example.com/image2.png)

**Figure 2** Proof of Theorem 20. \( w = yxx, |y| > |x| \), Case 1: the internal occurrence of \( y \) does not overlap with the prefix \( y \).

Case 1 In this case, \( x \) has an overlap \( u \) with itself (see Figure 2). Then there exist a suffix \( t \) of \( y \) and a prefix \( v \) of \( y \) such that \( x = tu = uv \). Clearly, \( t \neq v \), otherwise \( x \) would not be primitive. By Lemma 10 we have \( t = (pq)^m, v = (qp)^m \) and \( u \in (pq)^\ast p \). Now, the internal occurrence of \( y \) is a prefix of \( xv = uvv \) and it is longer than \( x = vu \), so it is of the form \( y = uvv' \) for some prefix \( v' \) of \( v \). Now, \( t \) is a suffix of \( y \) such that \( |t| = |v| > |v'| \). Therefore, since \( pq \) cannot occur internally in \( ppq \) (as, by Lemma 10 \( pq \) is primitive), and \( pq \neq q \), we have that \( v' \) must be of the form \( v' = (qp)^i q \) for some \( i \). Thus, both \( x \) and \( y \) belong to \( \{p, q\}^\ast \), against the hypothesis that \( \{x, y\} \) is a primitive pair.
Case 2. Let us now suppose that $y$ has an overlap $u$ with itself (see Figure 3). Then we can write $y = tu = uv$, with $u \neq v$ since $y$ is primitive, and in this case $x$ is a suffix of $t$ and a prefix of $v$. By Lemma 10 we have $t = (pq)^m$, $v = (qp)^m$ and $u \in (pq)^*p$. It follows that $x$ has the form $(qp)^q$. Thus, both $x$ and $y$ belong to $\{p,q\}^*$, against the hypothesis that $(x,y)$ is a primitive pair.

Let now $|y| \leq |x|$.

The internal occurrence of $xy$ must begin before the end of the prefix $y$ of $w$, otherwise $x$ would have an internal occurrence in $xx$, against the hypothesis that $x$ is primitive. So, $x$ has an overlap $u$ with itself (see Figure 4).

As in Case 1 there exist a suffix $t$ of $y$ and a prefix $v$ of $y$ such that $x = tu = uv$. Clearly, $t \neq v$, otherwise $x$ would not be primitive. By Lemma 10 we have $t = (pq)^m$, $v = (qp)^m$ and $u \in (pq)^*p$. Now, the internal occurrence of $y$ is a prefix of $vx = uv$ but now it is shorter than $x = vu$, as $|y| \leq |x|$, so it is of the form $y = vu'$ for some prefix $u'$ of $u$. Now, since $pq$ cannot occur internally in $pqpq$ (as, by Lemma 10, $pq$ is primitive), and $pq \neq qp$, and since $y$ ends in $t$, we have that $u'$ must be of the form $u' = (pq)^i$ for some $i$. Thus, both $x$ and $y$ belong to $\{p,q\}^*$, against the hypothesis that $(x,y)$ is a primitive pair.

The case $w = yxx$ is now proved.

The proof of the case $w = yyx$ is analogous by symmetry.

\[\text{\because} \]