On the Maximal Number of Cubic Subwords in a String[⋆]

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Abstract. We investigate the problem of the maximum number of cubic subwords (of the form www) in a given word. We also consider square subwords (of the form ww). The problem of the maximum number of squares in a word is not well understood. Several new results related to this problem are produced in the paper. We consider two simple problems related to the maximum number of subwords which are squares or which are highly repetitive; then we provide a nontrivial estimation for the number of cubes. We show that the maximum number of squares xx such that x is not a primitive word (nonprimitive squares) in a word of length n is exactly $\lfloor \frac{n}{2} \rfloor - 1$, and the maximum number of subwords of the form x^k, for $k \geq 3$, is exactly $n - 2$. In particular, the maximum number of cubes in a word is not greater than $n - 2$ either. Using very technical properties of occurrences of cubes, we improve this bound significantly. We show that the maximum number of cubes in a word of length n is between $\frac{45}{100}\,n$ and $\frac{4}{5}\,n$.

1   Introduction

A repetition is a word composed (as a concatenation) of several copies of another word. The exponent is the number of copies. We are interested in natural exponents higher than 2. In [4] the authors considered also exponents which are not integer.

In this paper we investigate the bounds for the maximum number of highly repetitive subwords in a word of length n. A word is highly repetitive iff it is of the form x^k for some integer k greater than 2. In particular, cubes w^3 and squares x^2 with nonprimitive x are highly repetitive.

The subject of computing maximum number of squares and repetitions in words is one of the fundamental topics in combinatorics on words [16,19] initiated by A. Thue [25], as well as it is important in other areas: lossless compression, word representation, computational biology etc.

The behaviour of the function $squares(n)$ of maximum number of squares is not well understood, though the subject of squares was studied by many authors, see [7,8,15]. The best known results related to the value of $squares(n)$ are, see [11,13,14]:

$$n - o(n) \leq squares(n) \leq 2n - O(\log n)$$

In this paper we concentrate on larger powers of words and show that in this case we can have much better estimations. Let $cubes(n)$ denote the maximum number of cubes in a word of length n. We show that:

$$\frac{45}{100} n \leq cubes(n) \leq \frac{4}{5} n$$

There are known efficient algorithms for the computation of integer powers in words, see [1,3,9,20,21].

The powers in words are related to maximal repetitions, also called *runs*. It is surprising that the bounds for the number of runs are much tighter than for squares, this is due to the work of many people [2,5,6,12,17,18,22,23,24].

Our main result is a new estimation of the number of cubic subwords. We use a new interesting technique in the analysis: the proof of the upper bound is reduced to the proof of an invariant of some abstract algorithm (in our invariant lemma). There is still some gap between upper and lower bound but it is much smaller than the corresponding gap for the number of squares.

2   Basic Properties of Highly Repetitive Subwords

We consider *words* over a finite alphabet A, $u \in A^*$; by ε we denote an empty word; the positions in a word u are numbered from 1 to $|u|$. For $u = u_1 \ldots u_k$, by $u[i..j]$ we denote a *subword* of u equal to $u_i \ldots u_j$. We say that a positive integer p is a *period* of a word $u = u_1 \ldots u_k$ if $u_i = u_{i+p}$ holds for $1 \leq i \leq k - p$. If $w^k = u$ (k is a non-negative integer) then we say that u is the kth power of the word w.

The *primitive root* of a word u, denoted $root(u)$, is the shortest word w, such that $w^k = u$ for some positive k. We call a word u *primitive* if $root(u) = u$, otherwise it is called *nonprimitive*. It can be proved that the primitive root of a word u is the only primitive word w, such that $w^k = u$ for some positive k. A *square* is the 2nd power of some word, and an *np-square* (a nonprimitive square) is a square of a word, that is **not** primitive. A *cube* is a 3rd power of some word.

In this paper we focus on the last occurrences of subwords. Hence, whenever we say that word u *occurs at position i* of the word v we mean its **last** occurrence, that is $v[i..i+|u|-1] = u$ and $v[j..j+|u|-1] \neq u$ for $j > i$. The following lemma is used extensively throughout the article.

Lemma 1 (Periodicity Lemma [10,19]). *If a word of length n has two such periods p and q, that $p + q \leq n + \gcd(p, q)$, then $\gcd(p, q)$ is also a period of the word.*
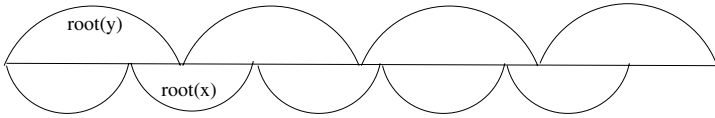
Fig. 1. The situation when one hr-word is a (long) prefix of another hr-word implies that $root(x) = root(y)$, consequently x is a suffix of y

We often use, so called, weak version of this lemma, where we only assume that $p + q \leq n$.

A word is said to be *highly repetitive* (hr-word) if it is a kth power of a nonempty word, for $k \geq 3$.

Lemma 2. *If a hr-word x is a prefix of a hr-word y and $|x| \geq |y| - |root(y)|$, then x is also a suffix of y.*

Proof. Due to the periodicity lemma, both words have the same smallest period and it is a common divisor of the lengths of their primitive roots, see Figure 1. Consequently, we have $root(x) = root(y)$ and x is a suffix of y. □

Lemma 3. *Assume that x and y are two hr-words, where $y = z^3$ and x is a subword of y starting at position $j \leq \left\lceil \frac{|root(z)|}{2} \right\rceil + 1$ and ending at position $k > |z^2|$. Then, $|root(x)| = |root(y)|$.*

Proof. Let $x = w^k$, for some $k \geq 3$. First, let us note that if the hypothesis of the lemma holds, then $|x| > \frac{3}{2}|z|$ — this can be verified by careful examination of simple cases: for even and odd values of $|z|$. Let us also observe, that $|root(x)|$ and $|root(y)|$ are both periods of x. Moreover:

$$|x| = |w^k| = |w| + \frac{k-1}{k}|x| \geq |w| + \frac{2}{3}|x| > |w| + |z| \geq |root(x)| + |root(y)|$$

From this, by the periodicity lemma, we obtain that $g = \gcd(|root(x)|, |root(y)|)$ is also a period of x. However, $root(x)$ and $root(y)$ are subwords of x, so $g = |root(x)| = |root(y)|$. □

3   Some Simple Bounds

In this section we give some simple estimations of the number of square subwords with nonprimitive roots and cubic subwords.

Lemma 4. *Let u be a word. Let us consider highly repetitive subwords of u of the form v^k, for $k \geq 3$ and v primitive. For each such subword we consider its (last) occurrence in u. For each position i in u, at most one such subword can have its (last) occurrence at position i.*

Proof. Let us assume, that we have two different hr-words x and y with their last occurrences starting at position i, and let us assume that x is shorter. Then, we have: $|x| \geq |y| - |root(y)|$, otherwise the considered occurrence of x would not be the last one.

Now we can apply Lemma 2 — x is not only a prefix of y, but also its suffix. Hence, x appears later in the text and the last occurrence of x in u does not start at position i. This contradiction proves, that the assumption that the last occurrences of x and y start at position i is false. $\square$

The following fact is a straightforward consequence of Lemma 4.

Theorem 1. *The maximum number of highly repetitive subwords of a word of length $n \geq 2$ is exactly $n - 2$.*

Proof. From Lemma 4 we know, that at each position there can be at most one last occurrence of a nonempty hr-word. Moreover, the minimum possible length of such a word is 3. So, it cannot occur at positions n and $n - 1$. On the other hand, this upper bound is reached by the word a^n. $\square$

As a corollary, we obtain a simple upper bound for the number of cubes, since cubes are hr-words.

Corollary 1. *Let us consider a word u of length n. The number of nonempty cubes appearing in u is not greater than $n - 2$.*

We improve this upper bound substantially in the next section. However, it requires a lot of technicalities. Another implication of Theorem 1 is a tight bound for the number of np-squares.

Theorem 2. *Let u be a word of length n. The maximum number of nonempty np-squares appearing in u is exactly $\left\lfloor \frac{n}{2} \right\rfloor - 1$.*

Proof. Each nonempty np-square can be viewed as v^{2i} for some nonempty primitive v and $i \geq 2$. However, each such np-square contains a subword v^{2i-1}, which is not an np-square, but still a hr-word. Hence, the number of nonempty subwords of the form v^{2i-1} (for primitive v and $i \geq 2$), appearing in the given word, is not smaller than the number of nonempty np-squares.

Please observe, that Theorem 1 limits the total number of both subwords of the form v^{2i} and v^{2i-1}, by $n-2$. Hence, the total number of nonempty np-squares appearing in the given word is not greater than $\frac{n}{2} - 1$, and since it is integer, it is not greater than $\left\lfloor \frac{n}{2} \right\rfloor - 1$. On the other hand, this upper bound is reached by the word a^n. $\square$

4   The Number of Cubic Subwords

In this section we show, that the upper bound on the number of different cubes in a word of length n is $\frac{4}{5}n$. We also show example words containing $0.45n$ different cubes. The following lemma states the main idea of the proof of the upper bound.

Lemma 5. *Let v^3 and w^3 be two nonempty cubes occurring in a word u at positions i and j respectively, such that:*

$$i < j \leq i + \left\lceil \frac{|root(v)|}{2} \right\rceil$$

Then either $|root(w)| = |root(v)|$ or $|root(w)| \geq 2 \cdot |root(v)| - (j - i - 1)$.

Proof. Let us denote $p = |root(v)|$, $q = |root(w)|$, and let k be the position of the last letter of w^3.

Let us first consider the case, when the (last) occurrence of w^3 is totally inside v^3. Please note, that k must then be within the last of the three v's, since otherwise w^3 would occur in u at position $j + p$ or further (see also Fig. 2). Hence, due to Lemma 3, we obtain $q = p$.

In the opposite case, let x be the maximal prefix of w^3 that lays inside v^3. If $p \neq q$ then, by the periodicity lemma, $p + q$ must be greater than $|x|$ (please note that if $p + q \leq |x|$ then obviously both $root(v)$ and $root(w)$ are subwords of x). Therefore:

$$p + q > |x| > |v^3| - (j - i) \geq 3p - (j - i)$$

and hence $q \geq 2p - (j - i) + 1$. $\square$

Let us introduce a notion of *p-occurrence*.

Definition 1. *A p-occurrence is the (last) occurrence of a cube with primitive root of length p.*

It turns out, that the primitive roots of cubes appearing close to each other cannot be arbitrary. It is formally expressed by the following lemma.

Lemma 6. *Let $a_1, a_2, \ldots, a_{p+1}$ be an increasing sequence of positions in a word u, such that $a_{j+1} \leq a_j + p$ for $j = 1, 2, \ldots, p$. It is not possible that there are p-occurrences at all these positions.*

Proof. Let us assume, to the contrary, that at each of the positions $a_1, a_2, \ldots, a_{p+1}$ there is a p-occurrence. Please note, that the inequalities from the hypothesis of the lemma imply that the primitive roots of cubes occurring at these positions are all cyclic rotations of each other. There are only p different
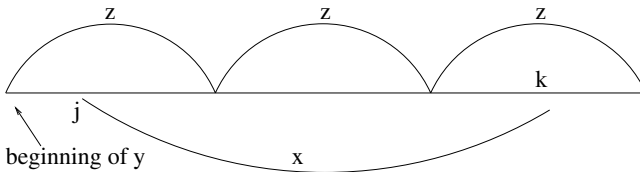

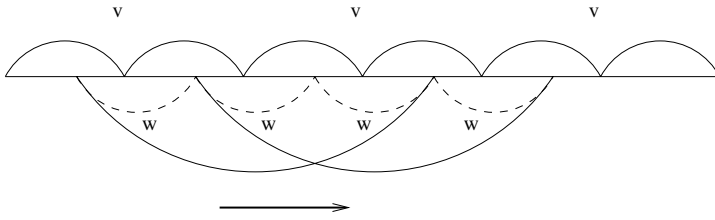**Fig. 2.** The situation from Lemma 3

Fig. 3. Positions of cubes v^3 and w^3 for the case $l < k$: a_{j+1} is not the last occurrence of w^3
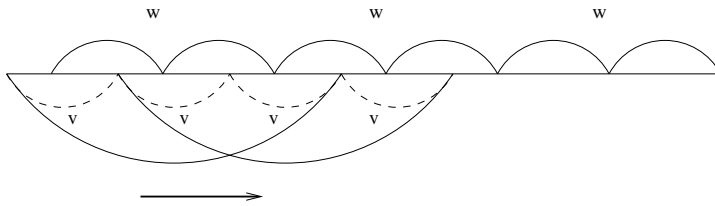

Fig. 4. Positions of cubes v^3 and w^3 for the case $k < l$: a_j is not the last occurrence of v^3

rotations of such primitive roots, so due to the pigeonhole principle, some two of them must be equal.

It suffices to show, that all these cubes have the same length, because then two of them must be equal, and one of them is not the last occurrence of the cube.

So, let us assume to the contrary, that some of the considered cubes have different lengths. Let a_j and a_{j+1} be such two considered positions, that cubes (v^3 and w^3 respectively) occurring at these positions have different lengths ($3kp$ and $3lp$ respectively, for $k \neq l$). Let us consider two cases. If $l < k$, then $3kp - 3lp \geq 3p$, and w^3 occurs in u at position $a_{j+1} + p$ or further.

On the other hand, if $k < l$, then $3lp - 3kp \geq 3p$ and v^3 appears in u at position $a_j + p$ or further. So, in both cases we obtain a contradiction. Hence it is not possible, that the lengths of the cubes differ. □

Let us introduce a notion of independent prefixes.

Definition 2. *We say that v is the* independent prefix *of u if it is the shortest prefix of u, that is:*

1. *a 1-letter word, if there is no occurrence of a cube at the first position of u, or otherwise*
2. *such a word v, for which the last occurrence of a cube in u, that starts within v is a q-occurrence (for some $q \geq 1$), and after this occurrence there are exactly $\left\lceil \frac{q}{2} \right\rceil$ positions (within v) without any occurrences of cubes (in u).*

It is not obvious, that the above definition is valid. Therefore, we prove the following lemma:

Lemma 7. *For every word u, there exists an independent prefix v of u.*

Proof. If there is no occurrence of a cube at the first position of u, then obviously $v = u[1..1]$. In the opposite case, let us assume that the independent prefix does not exist. Let q be the maximum such value, that some q-occurrence exists in u, and let i be the rightmost position in u, that contains a q-occurrence. From Lemma 5, $\lceil \frac{q}{2} \rceil$ positions following i do not contain any occurrences of cubes. So, the prefix $u[1..i + \lceil \frac{q}{2} \rceil]$ satisfies the properties of an independent prefix — a contradiction. □

Lemma 8. *Let v be the independent prefix of u. The number of different nonempty cubes that occur in u and start within v is not greater than $\frac{4}{5}|v|$.*

Proof. Please note, that if v satisfies the first condition of Definition 2, then the conclusion trivially holds. Therefore, from now on we assume that $|v| > 1$.

Let c_i be a sequence describing the occurrences starting within v: $c_i = 0$ iff there are no occurrences in position $v[i]$, and $c_i = q$ iff there is a q-occurrence in position $v[i]$. Please note that:

a) Let $i < j$ be such indices, that $c_i, c_j > 0$ and $c_{i+1} = \ldots = c_{j-1} = 0$. If $j - i > \lceil \frac{c_i}{2} \rceil$, then the prefix of u of length $i + \lceil \frac{c_i}{2} \rceil$ or shorter is an independent prefix of u — a contradiction. So, for any such i and j we have $j - i \le \lceil \frac{c_i}{2} \rceil$.
b) From Lemma 5 we obtain that $c_j \ge 2c_i - (j - i - 1)$.
c) From Lemma 6 and due to a) we have that no $q + 1$ consecutive positive elements of c can be equal q.

From now on, we abstract from the actual word u, and focus only on the properties of sequence c. We show, that the ratio R of non-zero elements of c to the length of c does not exceed $\frac{4}{5}$.

Let us observe that if c contains such a pair of equal elements $c_i = c_j > 0$, that all the elements between them are equal zero, then all the elements between c_i and c_j can be removed from c without decreasing R. Also, if c contains a subsequence of consecutive elements equal to q ($q > 0$) of length less than q then this subsequence can be extended to length q without decreasing R. Let c' be a sequence obtained from c by performing the described modification steps (as many times as possible). Please note that none of these steps violates properties b) or c). We will show, that even for c' the ratio of non-zero elements does not exceed $\frac{4}{5}$.

Every possible sequence c' can be generated by the (nondeterministic) pseudocode shown below. The following variables are used in the pseudocode:

- p — the value of the last positive element of c'
- len — the length of the sequence c' without $\lceil p/2 \rceil$ trailing zeros
- occ — the number of positive elements in c'
- l — the gap between consecutive different positive elements of c'
- α — the difference between the actual value of a positive element of c' and the lower bound from Lemma 5.

$$3\ 3\ 3\ 0\ \underbrace{5\ldots5}_{5\text{ times}}\ 0\ 0\ \underbrace{20\ldots20}_{20\text{ times}}\ \underbrace{0\ldots0}_{6\text{ times}}\ \underbrace{34\ldots34}_{34\text{ times}}\ \underbrace{0\ldots0}_{17\text{ times}}$$
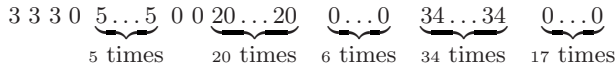
Fig. 5. An example of sequence c'. The length of the sequence is 88 and it contains 62 positive elements. The ratio is $62/88 \approx 0.70 < 4/5$.

Each step of the **repeat-until** loop corresponds to extending sequence c', i.e. adding l zeros and p elements of value p.

Note that the algorithm specified by the pseudocode is nondeterministic in a few different aspects — the initial value of p, the number of steps of the **repeat-until** loop and values of l and α.

$p :=$ some positive integer;
$occ := p;$ $len := p;$
output: $\underbrace{p\ldots p}_{p\text{ times}}$
repeat
    Invariant $I(p, occ, len) : \frac{occ}{len + \frac{p}{2}} \le \frac{4}{5}$.
    $l :=$ some integer from interval $[0, \lceil\frac{p}{2}\rceil)$;
    $\alpha :=$ some non-negative integer;
    $p := 2p - l + \alpha;$
    $occ := occ + p;$
    $len := len + l + p;$
    output: $\underbrace{0\ldots0}_{l\text{ times}} \underbrace{p\ldots p}_{p\text{ times}}$
until done

In order to prove the $\frac{4}{5}$ bound, we need to show that inequality

$$\frac{occ}{len + \lceil\frac{p}{2}\rceil} \le \frac{4}{5}$$

holds for every possible execution of the above pseudocode. But this inequality is a consequence of the fact that $I(p, occ, len)$ is an invariant of the **repeat-until** loop (Lemma 9). □

Lemma 9 (Invariant Lemma). *Inequality $I(p, occ, len)$:*

$$\frac{occ}{len + \frac{p}{2}} \le \frac{4}{5}$$

*is an invariant of the **repeat-until** loop from the above pseudocode.*

Proof. It is easy to check that before the first execution of the **repeat-until** loop inequality $I(p, occ, len)$ holds. Therefore, we only need to prove that if

n	word	#cubes	ratio
20	01110101011011011000	7	0.35
30	000000110110110101101011010101	11	0.36
40	1101101101110111011100010001000100100100	16	0.40
50	11111111110010010010100101001010100101010010101000	20	0.40
60	101001010010100101010010100101010010100101001010 1001010100	25	0.41
70	00000011011011010110101101010110101101010110101101 01011010101101010111	30	0.42
80	11011011010110110101101101011010110101011010110101 011010110101011010101101010111	34	0.42
90	11101101101110110110111011011011101101011101101110111 01101110110110111011011101101011011101110	40	0.44
100	1000101010010101001010100101001010100101001010100 1 0100101001010100101001010010101001010010100101001010111	44	0.44
200	0000100010001000100010001000100010001000100001000100 0010001000100010001000100001000100001000100010000 1000100010000100010000100010001000010001000010000100010 0010000100010000100010000100010000110111011101110	91	0.45

Fig. 6. Examples of words with high number of distinct cubic subwords

$I(p, occ, len)$ holds then $I(p', occ', len')$ also holds, where p', occ' and len' are the values obtained as a result of a single step of the **repeat-until** loop, i.e.:

$$p' = 2p - l + \alpha, \quad occ' = occ + 2p - l + \alpha, \quad len' = len + 2p + \alpha$$

Let us restate $I(p', occ', len')$ equivalently in the following way:

$$5 \cdot occ + 10p - 5l + 5\alpha \leq 4 \cdot len + 8p + 4\alpha + 4 \cdot \frac{2p - l + \alpha}{2} \qquad (1)$$

Since $I(p, occ, len)$ can be expressed as $5 \cdot occ \leq 4 \cdot len + 4 \cdot \frac{p}{2}$, in order to show (1), it is sufficient to prove that:

$$10p - 5l + 5\alpha \leq 8p + 4\alpha + 2 \cdot (2p - l + \alpha) - 2p \qquad (2)$$

As a result of some rearrangement, (2) can be expressed as $0 \leq 3l + \alpha$ and this inequality trivially holds. □

Theorem 3. *The number of different nonempty cubes that occur in a word of length n is not greater than $\frac{4}{5}n$.*

Proof. This theorem is a consequence of Lemmas 7 and 8 — it can be proved by simple induction on n, where the inductive step consists of removing the independent prefix. □

Theorem 4. *For infinitely many positive integers n there exist words x of length n with at least $0.45 \cdot n$ different nonempty cubic subwords.*

Proof. A trivial lower bound on the number of different cubic subwords is the word a^n with $\lfloor \frac{n}{3} \rfloor$ cubic occurrences. The table presented in Figure 6 contains examples of some words with higher number of cubic subwords. These words have been computed using extensive computer experiments. For example, we have found a word w of length 200 over binary alphabet containing 91 different nonempty cubic subwords. For any positive integer k we can construct a word $x = w_1 w_2 \ldots w_k$ (over the alphabet $\{0, 1, \ldots, 2k-1\}$), where w_i is a word created from w by replacing all occurrences of letter 0 by $2(i-1)$, and 1 by $2i-1$. Such word x has length $200k$ and contains at least $91k$ cubic subwords (91 in each subword w_i). This gives a ratio $91/200 \cdot n > 0.45 \cdot n$.   □

5   Conclusions

In this paper we prove a tight bound for the number of nonprimitive squares in a word of length n. Unfortunately, this does not improve the overall bound of the number of squares — the main open problem is improving the bound for primitive squares.

We also give some estimations of the number of cubes in a string of length n. Although they are much better than the best known estimations for squares in general, they can still be subject to improvement — both the lower and the upper bound do not seem to be tight.

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