

# Improved Bounds on the Maximum Number of Distinct Squares in Circular Words

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## Abstract

We investigate the asymptotic growth of function  $\text{CS}(n)$ , which maps  $n$  to the maximum number of distinct squares in a circular word of length  $n$  (that is, the maximum number of distinct squares of length at most  $n$  in a word  $ww$  of length  $2n$ ). We improve upon the lower bound of  $1.25n$  established by Amit and Gawrychowski [SPIRE 2017] and the straightforward upper bound of  $2n$ , which follows from the recent result of Brlek and Li [Comb. Theory, 2025] stating that there are fewer than  $n$  squares in standard (i.e., non-circular) words of length  $n$ . (Previously, Amit and Gawrychowski gave an upper bound of  $3\frac{2}{15}n$  using a weaker upper bound on squares in standard words.) Specifically, we show that  $\text{CS}(n) \leq \lceil 1.8n \rceil$  and that, for infinitely many  $n$ ,  $\text{CS}(n) \geq 1.5n - \mathcal{O}(\sqrt{n})$ .

For the lower bound, we exploit the combinatorial structure of Fibonacci words to construct a family of square-rich circular words. For the upper bound, we exploit density properties of the starting positions of long squares, adapting an approach of Amit and Gawrychowski.

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## 1 Introduction

The study of square and symmetric fragments of words is central in combinatorics and algorithms on words. A square is a word of the form  $uu$  for a word  $u$ . Here, we focus on square fragments of circular words. That is, for a standard word  $w$ , we study the square fragments that occur in any rotation of  $w$  or, equivalently, the square fragments of  $ww$  that are of length at most  $|w|$ .

The earliest result concerning squares in words is the construction of square-free ternary words of all lengths by Thue [19]. The analogue of this problem for circular words is more intricate. Currie [4] showed that square-free circular words over the ternary alphabet exist for all lengths except for 5, 7, 9, 10, 14, and 17 using a computer-aided proof. Shur [16] later gave a computer-free proof that also implied an exponential (in the length) lower bound on the number of such words of any fixed length.



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Let  $\text{SQ}(n)$  be the maximum number of distinct squares in a (standard) word of length  $n$ . Fraenkel and Simpson [7] proved that  $\text{SQ}(n) < 2n$  and conjectured that  $\text{SQ}(n) < n$ . The resolution of this conjecture took more than two decades. Milestone results include the upper bound of  $2n - \log n$  due to Ilie [9], the upper bound of  $\frac{11}{6}n$  due to Deza, Franek, and Thierry [5], and the upper bound of  $1.5n$  due to Thierry [18]. Finally, Brlek and Li [3] confirmed the Fraenkel-Simpson conjecture using a graph-theoretic approach, establishing that  $\text{SQ}(n) < n$ .

Let  $\text{CS}(n)$  denote the maximum number of distinct squares in a circular word of length  $n$ . The growth of  $\text{CS}(n)$  was first studied by Amit and Gawrychowski [1] who showed an upper bound of  $3\frac{2}{15}n$  and a lower bound of  $1.25n$  (for infinitely many  $n$ ). Note that this work was published when the best known upper bound for standard squares was  $\text{SQ}(n) \leq \frac{11}{6}n$ . Further, observe that the number of squares of length at most  $n$  in a word  $ww$  is at most  $\text{SQ}(2|w|)$ . The result of Brlek and Li [3] thus implies that  $\text{CS}(n) \leq \text{SQ}(2n) < 2n$ .

**Our results.** Here, we improve upon both the upper bound of  $2n$  that follows from [3] and the lower bound of  $1.25n$  from [1] for  $\text{CS}(n)$ . Specifically, we show that  $\text{CS}(n) \leq \lceil 1.8n \rceil$  for all  $n$  and that  $\text{CS}(n) \geq 1.5n - \mathcal{O}(\sqrt{n})$  for infinitely many  $n$ .

Our lower and upper bounds are presented in Section 3 and Section 4, respectively. Then, Section 5 discusses the limitations of our approach.

**Discussion.** As we remark at the end of Section 4, the proof of the  $3\frac{2}{15}n$  upper bound of Amit and Gawrychowski could be modified to yield an upper bound of  $\lceil \frac{13}{7}n \rceil$  by incorporating the upper bound of  $n$  for standard squares. However, the resulting argument remains technically involved. We establish a stronger upper bound of  $\lceil 1.8n \rceil$  and also a (still stronger) upper bound of  $\lceil \frac{11}{6}n \rceil$  which is considerably simpler.

## 2 Preliminaries

A word  $u = u[0] \cdots u[n-1]$  is a sequence of length  $|u| = n$  of letters from some alphabet. For any two integers  $i, j \in [0..|u|]$ ,  $u[i..j]$  and  $u[i..j+1)$  denote the fragment  $u[i] \cdots u[j]$  if  $i \leq j$  and the empty word otherwise. A fragment  $u[0..j]$  is called a *prefix* of  $u$ . A prefix of  $u$  is called a *proper prefix* of  $u$  if its length is smaller than  $n$ . A fragment  $u[i..n-1]$  is called a *suffix* of  $u$ .

We say that integer  $p \in [1..|u|]$  is a *period* of a word  $u$  if  $u[i] = u[i+p]$  for all  $i \in [0..|u|-p)$ . We denote the smallest period of  $u$  by  $\text{per}(u)$ . We say that  $u$  is *periodic* if  $\text{per}(u) \leq \frac{1}{2}|u|$ ; otherwise  $u$  is called *non-periodic*.

► **Lemma 1** (Periodicity Lemma [6]). *If a word  $u$  has periods  $p$  and  $q$  such that  $p + q \leq |u| + \gcd(p, q)$ , then  $\gcd(p, q)$  is also a period of  $u$ .*

A word  $u$  is called *primitive* if the equality  $u = v^k$  for a positive integer  $k$  implies that  $k = 1$ . Primitive words satisfy the following synchronization property that follows from the periodicity lemma: a primitive word  $u$  occurs in  $u^2$  only as a prefix and as a suffix.

For a word  $u$ , for any integer  $i \in [0..|u|]$ , we call  $u[i..|u|)u[0..i)$  a *rotation* of  $u$ .

For a word  $w$ , we denote by  $\mathbf{S}_n(w)$  the set of squares of length at most  $n$  that occur in  $w$ . Thus, the set of squares of a circular word  $w$  equals  $\mathbf{S}_n(w^2)$ , where  $n = |w|$ .

Fibonacci words are defined by the recurrence

$$F_0 = b, \quad F_1 = a, \quad F_t = F_{t-1}F_{t-2} \text{ for } t \geq 2.$$

The number of distinct squares in the (standard) word  $F_n$  is equal to  $2|F_{n-2}| - 2$ ; see [8]. As a warm-up, we show an exact bound on the number of squares in circular Fibonacci words.

► **Fact 2.** *If  $n \geq 2$ ,  $|\mathbf{S}_{|F_n|}(F_n F_n)| = |F_n| - 2$ .*

**Proof.** Every square in  $F_n$  is a square of a rotation of some shorter Fibonacci word; see [10, Theorem 2.3]. The same holds for  $F_n^2$  since  $F_n^2$  is a prefix of the infinite Fibonacci word for  $n \geq 3$ , and for  $n \leq 2$  it can be easily verified.

For  $n = 2$ , we have  $\mathbf{S}_{|F_n|}(F_n F_n) = \emptyset$  as expected. Assume  $n \geq 3$ . The set  $\mathbf{S}_{|F_n|}(F_n^2)$  does not contain  $F_0^2 = bb$  and  $F_{n-1}^2$  (because  $2|F_{n-1}| > |F_n|$ ). Let us show by induction that for all  $k \in [1..n-2]$ , each rotation of  $F_k^2$  occurs in  $F_n^2$ . Correctness in the base cases of  $n \in \{3, 4\}$  can be easily checked. Assume that  $n \geq 5$  and the property holds for  $n-1$ . By the hypothesis,  $F_{n-1}^2$  contains all rotations of  $F_k^2$  for  $k \in [1..n-3]$ . Since  $n \geq 4$ ,  $F_{n-1}^2$  is a prefix of  $F_n^2$ , so all these squares are also in  $\mathbf{S}_{|F_n|}(F_n^2)$ . Moreover,  $F_n$  has a suffix  $F_{n-2}$  and a prefix  $F_{n-2}^2$  (since  $n-2 \geq 3$ ). Hence,  $F_n^2$  has a fragment  $F_{n-2}^3$ , so each rotation of  $F_{n-2}^2$  occurs in  $F_n^2$ .

In total, we obtain  $|F_1| + |F_2| + \dots + |F_{n-2}| = |F_n| - 2$  squares. All these squares are different because each Fibonacci word is primitive. ◀

► **Example 3.** We have

$$F_2 = a b, F_3 = a b a, F_4 = a b a a b, F_5 = a b a a b a b a, F_6 = a b a a b a b a b a b a b.$$

For  $F_6$ , we have

$$\mathbf{S}_{13}(F_6) = \{a^2, (ab)^2, (ba)^2, (aba)^2, (aab)^2, (baa)^2, (abaab)^2, (baaba)^2\},$$

and

$$\mathbf{S}_{13}(F_6^2) = \mathbf{S}_n(F_6) \cup \{(aabab)^2, (ababa)^2, (babaa)^2\}.$$

In particular,  $F_6$  has  $8 = 2|F_3| - 2$  distinct squares, while the circular  $F_6$  contains  $11 = |F_6| - 2$  distinct squares in total.

### 3 Lower Bound

We use Fibonacci words as building blocks. For any word  $v$  of length at least two, let  $\mathbf{cut}(v) := v[0..|v|-2]$  be the word obtained from  $v$  by deleting its two last letters. Let  $\mathbf{ex}(v)$  denote the word  $v$  with the last two letter exchanged, that is,  $\mathbf{ex}(v) := \mathbf{cut}(v)v[|v|-1]v[|v|-2]$ .

► **Example 4.**  $\mathbf{cut}(abcde) = abc$  and  $\mathbf{ex}(abcd) = abdc$ .

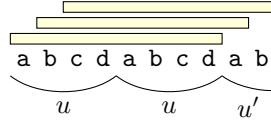
The following (folklore) property of Fibonacci words follows by a straightforward inductive argument.

► **Observation 5.** *For  $t \geq 2$ , we have  $\mathbf{cut}(F_t) = \mathbf{cut}(F_{t-2}F_{t-1})$  and  $\mathbf{ex}(F_t) = F_{t-2}F_{t-1}$ .*

The next observation follows directly from the synchronization property of primitive words; see Figure 1.

► **Observation 6** (Squares in periodic fragments).

- (a) *If  $u'$  is a proper prefix of a primitive word  $u$ , then  $uuu'$  contains  $|u'| + 1$  distinct squares of length  $|uu|$ .*
- (b)  *$u^k$  contains at least  $\lfloor \frac{k-1}{2} \rfloor |u|$  words that are rotations of words in  $\{u^{2j} \mid 1 \leq j \leq \frac{1}{2}k\}$  and are pairwise distinct.*



■ **Figure 1** Illustration of Observation 6(a). For the primitive word  $u = \text{abcd}$  and its proper prefix  $u' = \text{ab}$ , the word  $u^2u'$  contains  $|u'| + 1$  distinct squares of length  $|u^2|$ :  $(\text{abcd})^2$ ,  $(\text{bcda})^2$ ,  $(\text{cdab})^2$ .

Before describing our construction, we first identify the primitive roots of the squares under consideration. These roots correspond to rotations of squares of words of the following types.

► **Observation 7** (Primitive words). *For any  $i > 0$  and  $t \geq 1$ , the words  $F_{t-1}$ ,  $F_t^i F_{t-1}$ , and  $F_t^i F_{t-1} F_t$  are primitive.*

**Proof.** For any  $t \geq 1$ , words  $F_{t-1}$  and  $F_t^k F_{t-1}$  are standard Sturmian words for  $k \geq 1$ . Since every standard Sturmian word is primitive (cf. [15]), it follows that all words of the form  $F_{t-1}$  and  $F_t^i F_{t-1}$  are primitive. Moreover, since any rotation of a primitive word is primitive, the word  $F_t^i F_{t-1} F_t$  is primitive as its rotation  $F_t^{i+1} F_{t-1}$  is primitive. ◀

**The construction.** We define an infinite family of words. For any  $k, t \in \mathbb{Z}_+$ , let

$$\mathcal{W}_{k,t} := F_t^k F_{t-1} F_t^{k+1} F_{t-1} F_t^{k+2} F_{t-1}.$$

Note that  $\mathcal{W}_{k,t}$  is parametrized by both  $k$  and  $t$  (eventually, we will set  $k := |F_t|$ ), and let  $n := |\mathcal{W}_{k,t}|$ . For convenience, we express bounds on the lengths of fragments and the number of square fragments in terms of

$$\alpha := |F_t^k| = k|F_t|.$$

Note that we have

$$|\mathcal{W}_{k,t}| = (3k + 3)|F_t| + 3|F_{t-1}| = 3\alpha + 3|F_{t+1}|. \quad (1)$$

**Squares in  $\mathcal{W}_{k,t}$  and  $\mathcal{W}_{k,t}^2$ .** We show that the words  $\mathcal{W}_{k,t}$  are almost cubes (except the last two letters); see Figure 2 for an illustration.

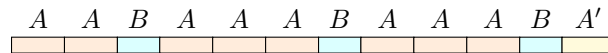
► **Lemma 8.** *For all  $k, t \in \mathbb{Z}_+$ , we have that  $\text{cut}(\mathcal{W}_{k,t}) = \text{cut}((F_t^k F_{t-1} F_t)^3)$ . Further,  $\mathcal{W}_{k,t}$  contains at least  $\alpha$  distinct squares which are rotations of  $(F_t^{k+1} F_{t-1})^2$ .*

**Proof.** We have

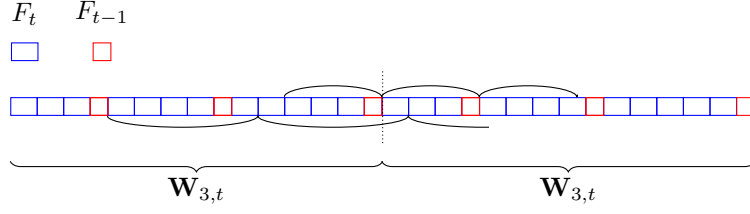
$$\mathcal{W}_{k,t} = F_t^k F_{t-1} F_t^{k+1} F_{t-1} F_t^{k+2} F_{t-1} = (F_t^k F_{t-1} F_t)(F_t^k F_{t-1} F_t) F_t^k F_{t-1} F_t.$$

By Observation 5,

$$\text{cut}(\mathcal{W}_{k,t}) = (F_t^k F_{t-1} F_t)(F_t^k F_{t-1} F_t)(F_t^k \text{cut}(F_{t-1} F_t)) = \text{cut}((F_t^k F_{t-1} F_t)^3).$$



■ **Figure 2** The structure of  $\mathcal{W}_{k,t}$  for  $k = 2$  and  $t \geq 2$ :  $\mathcal{W}_{k,t} = A^2 B A^3 B A^4 B$ , where  $A = F_t$  and  $B = F_{t-1}$ . We have  $\mathcal{W}_{k,t} = (AABA)^2 AABA'$ , where  $A' = \text{ex}(A)$ . We have  $\alpha = |F_t^k| = 2|A|$  and  $|\mathcal{W}_{2,t}| = 3\alpha + 3|AB|$ .



■ **Figure 3** Illustration of Lemma 9: Structure of  $\mathcal{W}_{k,t}^2$  for  $k = 3$ . The upper periodic fragment  $\mathcal{R}_1 = (F_t^k F_{t-1})^3$  in  $\mathcal{W}_{3,t}^2$  does not occur in  $\mathcal{W}_{3,t}$ . The lower periodic fragment is  $\mathcal{R}_2 = (F_t^{k+1} F_{t-1} F_t)^2 F_t^k$ . Together, these two periodic fragments contain at least  $2\alpha$  distinct squares of length at most  $n$ .

Hence,  $\text{cut}((F_t^k F_{t-1} F_t)^3)$  is a prefix of  $\mathcal{W}_{k,t}$ . Now,  $F_t^k F_{t-1} F_t$  is primitive due to Observation 7 and the second part of the statement follows by a direct application of Observation 6. ◀

► **Lemma 9.** *If  $t \geq 2$  and  $k > 0$ ,  $\mathcal{W}_{k,t}^2$  contains more than  $2\alpha$  distinct squares that are rotations of  $(F_t^k F_{t-1})^2$  and  $(F_t^{k+2} F_{t-1})^2$ .*

**Proof.** We denote  $\mathcal{R}_1 := (F_t^k F_{t-1})^3$  and  $\mathcal{R}_2 := (F_t^{k+1} F_{t-1} F_t)^2 F_t^k$ . We show that both  $\mathcal{R}_1$  and  $\mathcal{R}_2$  occur in  $\mathcal{W}_{k,t}^2$ ; see Figure 3. Then we obtain the statement using Observation 7 and Observation 6.

We first show that  $\mathcal{R}_1$  occurs in  $\mathcal{W}_{k,t}^2$ . The word

$$\mathcal{W}_{k,t}^2 = F_t^k F_{t-1} F_t^{k+1} F_{t-1} \left[ F_t^{k+2} F_{t-1} F_t^k F_{t-1} F_t^{k+1} \right] F_{t-1} F_t^{k+2} F_{t-1}$$

has a fragment equal to  $F_t^{k+2} F_{t-1} F_t^k F_{t-1} F_t^{k+1}$ , which in turn has a fragment equal to  $(F_t^k F_{t-1})(F_t^k F_{t-1}) F_t^k F_{t-1} = \mathcal{R}_1$ . Thus,  $\mathcal{W}_{k,t}^2$  contains more than  $\alpha$  distinct squares which are rotations of  $(F_t^k F_{t-1})^2$ .

Next, we show that  $\mathcal{R}_2$  occurs in  $\mathcal{W}_{k,t}^2$ . The word

$$\mathcal{W}_{k,t}^2 = F_t^k F_{t-1} \left[ F_t^{k+1} F_{t-1} F_t^{k+2} F_{t-1} F_t^k F_{t-1} F_t^{k+1} \right] F_{t-1} F_t^{k+2} F_{t-1}$$

contains a fragment equal to

$$F_t^{k+1} F_{t-1} F_t F_t^{k+1} F_{t-1} F_t F_t^{k-1} F_{t-1} F_t^{k+1}$$

which itself has a fragment equal to

$$(F_t^{k+1} F_{t-1} F_t) (F_t^{k+1} F_{t-1} F_t) F_t^{k-1} F_{t-1} F_t$$

which is equal to  $\text{ex}((F_t^{k+1} F_{t-1} F_t)^2 F_t^k F_{t-1})$ , since  $F_{t-1} F_t = \text{ex}(F_t F_{t-1})$ . Now, observe that  $\mathcal{R}_2 = (F_t^{k+1} F_{t-1} F_t)^2 F_t^k$  is a prefix of this fragment. Thus  $\mathcal{W}_{k,t}^2$  contains  $|F_t^k| + 1 = \alpha + 1$  distinct squares which are rotations of  $(F_t^{k+1} F_{t-1} F_t)^2$ .

Since  $F_t^k F_{t-1}$  and  $F_t^{k+2} F_{t-1}$  have different lengths, all considered square fragments are distinct and this concludes the proof. ◀

► **Lemma 10.** *If  $k \leq |F_t|$  then  $\mathcal{W}_{k,t}$  contains at least  $\alpha - \mathcal{O}(|F_t|)$  distinct squares which are rotations of  $(F_t^j F_{t-1})^2$  for  $0 < j < k$ .*

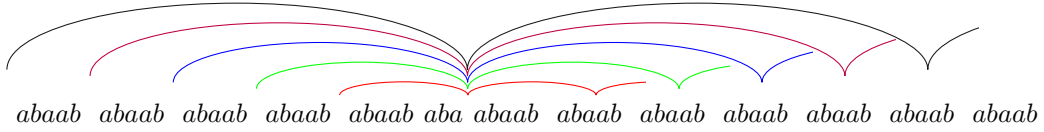
**Proof.** The word  $\mathcal{W}_{k,t}$  contains the fragment  $F_t^{k+1}F_{t-1}F_t^{k+2}$ ; see Figure 4. For each  $j \leq k$  it contains the fragment

$$F_t^j F_{t-1} F_t^{j+2} = \boxed{F_t^j F_{t-1} F_t^j F_{t-1} F_{t-2} F_{t-1}} F_{t-2} = F_t^j F_{t-1} F_t^j F_{t-1} \mathbf{ex}(F_{t-1} F_{t-2}) F_{t-2},$$

which contains the fragment  $(F_t^j F_{t-1})^2 \mathbf{cut}(F_t)$ .

By Observations 6 and 7, each such fragment,  $(F_t^j F_{t-1})^2 \mathbf{cut}(F_t)$ , contains  $|\mathbf{cut}(F_t)| + 1 = |F_t| - 1$  distinct squares that are rotations of  $(F_t^j F_{t-1})^2$ .

Summing over all  $0 < j < k$ , we obtain at least  $(|F_t| - 1) \cdot (k - 1) = \alpha - \mathcal{O}(|F_t|)$  distinct squares of the claimed form.  $\blacktriangleleft$



■ **Figure 4** Illustration of Lemma 10. For  $k = 4$ ,  $t = 4$ , let  $A = F_t = \text{abaab}$ ,  $B = F_{t-1} = \text{aba}$ , and  $C = \mathbf{cut}(F_t) = \text{aba}$ . Then  $\mathcal{W}_{k,t}$  contains the fragment  $F_t^k F_{t-1} F_t^{k+2}$ , which in turn contains the fragments  $(A^j B)^2 C$ , for  $1 \leq j \leq k$ . Each of these fragments implies  $|C| + 1 = |F_t| - 1$  squares. Altogether (including the case  $j = 0$ ), they contain  $(|F_t| - 1) \cdot k + |F_{t-1}|$  squares, but Lemma 10 excludes the squares generated for  $j = 0$  and  $j = k$  to avoid double counting.

The fact that  $F_t^{k+2}$  occurs in  $\mathcal{W}_{k,t}$  and Observations 6 and 7 imply the following:

► **Lemma 11.**  $\mathcal{W}_{k,t}$  contains at least  $\frac{1}{2}\alpha$  distinct squares that are rotations of the words in  $\{F_t^{2j} \mid 1 \leq j \leq \frac{k+2}{2}\}$ .

We are now ready to prove the main result of this section.

► **Theorem 12.** There are infinitely many integers  $n$  for which  $\text{CS}(n) \geq 1.5n - \mathcal{O}(\sqrt{n})$ .

**Proof.** Let us set  $k := |F_t|$ . Then  $\alpha = k^2$  and  $|F_t| = \mathcal{O}(\sqrt{n})$ . From Equation (1), the length of  $\mathcal{W}_{k,t}$  is  $n = 3\alpha + \mathcal{O}(\sqrt{n})$  and hence  $\alpha = \frac{1}{3}n - \mathcal{O}(\sqrt{n})$ .

By Lemmas 8–11, the word  $\mathcal{W}_{k,t}^2$  contains at least  $4.5\alpha - \Theta(|F_t|)$  squares (of length at most  $n$ ). They are all distinct. Indeed, the squares from Lemmas 8–10 are rotations of  $(F_t^j F_{t-1})^2$ , for different  $j \in [1..k+2]$ , so they have different lengths for different  $j$ . The squares from Lemma 11 are of the form  $(F_t^j)^2$  for  $j \leq k$ , and we have  $|F_t^{j-1} F_{t-1}| < |F_t^j| < |F_t^j F_{t-1}|$ .

Therefore, the circular word  $\mathcal{W}_{k,t}$  contains

$$4.5 \cdot \left(\frac{1}{3}n - \mathcal{O}(\sqrt{n})\right) = 1.5n - \mathcal{O}(\sqrt{n})$$

distinct squares, as required.  $\blacktriangleleft$

## 4 Upper Bound

Let us fix a word  $w$  of length  $n$ . We denote  $\tilde{w} = ww$ . Our aim is to show that  $|\mathbf{S}_n(\tilde{w})| \leq \lceil 1.8n \rceil$ .

**High-level idea of the proof.** If there exists a fragment (a  $\delta$ -window) of  $w^\infty$  of (small) length  $\delta$  that contains no starting position of a long square, then it is easy to show that there are at most  $2n - \delta$  distinct squares in the circular word  $w$ . If no such fragment exists, we call  $w$   $\delta$ -dense. Hence, we reduce the problem to showing that primitive  $\delta$ -dense words do

not exist – a simple upper bound of  $1.5n$  can be shown for non-primitive words. We view a square  $uu$  as a “transporter” which shifts long fragments of  $w$  by  $|u|$  positions (from the first copy of  $u$  to the second one). By choosing a long non-periodic fragment (called a *sample*)  $s$ , we consider only those distances  $|u|$  that correspond to the distances between occurrences of the sample in  $ww$  which start in the first copy of  $w$ . The number of these occurrences is very small (bounded by a constant). Then, using samples, we show that if  $w$  is primitive, then  $w$  is not  $\delta$ -dense.

► **Observation 13.** If  $w'$  is a rotation of  $w$ , then  $\mathbf{S}_n(ww) = \mathbf{S}_n(w'w')$ .

► **Lemma 14.** If  $w'$  is a rotation of  $w$  that is not primitive, then  $|\mathbf{S}_n(\tilde{w})| \leq 1.5n$ .

**Proof.** Suppose  $w' = u^k$  for some integer  $k \geq 2$ . Then  $\mathbf{S}_n(\tilde{w}) = \mathbf{S}_n(w'w') = \mathbf{S}_n(uw')$ . Consequently, due to [3], we have  $|\mathbf{S}_n(\tilde{w})| = |\mathbf{S}_n(uw')| \leq |u| + |w| = (1 + \frac{1}{k})n$ . Since  $k \geq 2$ , it follows that  $|\mathbf{S}_n(\tilde{w})| \leq 1.5n$ . ◀

► **Corollary 15.** If  $\tilde{w}$  contains a square of length exactly  $n$ , then  $|\mathbf{S}_n(\tilde{w})| \leq 1.5n$ .

By the above corollary, we may henceforth assume that  $w$  is primitive and  $\tilde{w}$  does not contain any square of length  $n$ .

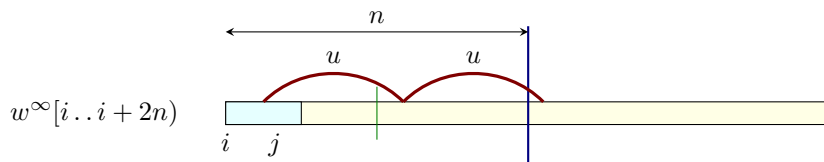
► **Remark 16.** Circular words that are themselves squares can still contain many squares. It was shown in [1] that there exists an infinite family of words  $w_k$ , each of which is a square, such that  $\mathbf{S}_n(w_k w_k) \geq 1.25|w_k| - o(|w_k|)$ .

► **Definition 17.** Let  $w$  be a word of length  $n$ . A square fragment  $uu$  starting at position  $j$  in  $w^\infty$  is called a  $\delta$ -square fragment with respect to an interval  $[i \dots i + \delta)$  if

$$i \leq j < i + \delta \text{ and } n - (j - i) < |uu| < n. \quad (2)$$

Observe that if  $j < \delta$  is the last occurrence in  $ww$  of a square  $uu$ , then  $uu$  is a  $\delta$ -square with respect to the interval  $I = [0 \dots \delta)$ .

► **Definition 18.** A word  $w$  is called  $\delta$ -dense if, for every length- $\delta$  fragment  $I$  of  $w^\infty$ , there exists a  $\delta$ -square fragment with respect to  $I$ . (See Figure 5.)



■ **Figure 5** Illustration of the notion of  $\delta$ -density. The shown word is a prefix of  $w^\infty[i \dots \infty)$ . Here,  $uu$  is a  $\delta$ -square fragment with respect to the interval  $I = [i \dots i + \delta)$  (shown in blue): there exists a position  $j$  in the interval  $I$  where a square  $uu$  starts and satisfies  $|uu| + (j - i) > n$ . The word  $w$  is  $\delta$ -dense if such a square  $uu$  exists for each interval  $[i \dots i + \delta)$  with  $i \in \mathbb{Z}_+$ .

We first consider the easy case when  $\tilde{w}$  is not  $\delta$ -dense.

► **Lemma 19** (Upper bound for words that are not  $\delta$ -dense). If  $\tilde{w}$  is not  $\delta$ -dense, where  $0 < \delta \leq \frac{1}{2}n$ , then  $|\mathbf{S}_n(\tilde{w})| \leq 2n - \delta$ .

**Proof.** By Corollary 15, if  $\tilde{w}$  contains a square fragment of length exactly  $n$ ,  $|\mathbf{S}_n(\tilde{w})| \leq 1.5n$ . Henceforth we assume that  $\tilde{w}$  does not have such a fragment. Since  $\tilde{w}$  is not  $\delta$ -dense, by the definition, there exists an interval  $I = [i \dots i + \delta)$  in  $w^\infty$  such that no  $\delta$ -square fragment exists with respect to  $I$ . That is, for every square fragment  $uu$  starting at some position  $j \in I$ ,  $|uu| < n - (j - i)$ . Equivalently, the longest square starting at any position  $q \in I$  has length at most  $n - (q - i)$ . After a rotation (cf. Observation 13), we may assume that  $i = 0$ , so that  $I = [0 \dots \delta)$ . Now, let us consider the suffix  $\tilde{w}'$  of  $\tilde{w}$  of length  $2n - \delta$ . Every square fragment of  $\tilde{w}$  occurs entirely within  $\tilde{w}'$ . Therefore, all distinct squares appear in a fragment of length  $2n - \delta$ . The combination of this fact and the result of [3] implies that  $|\mathbf{S}_n(\tilde{w})| \leq 2n - \delta$ . ◀

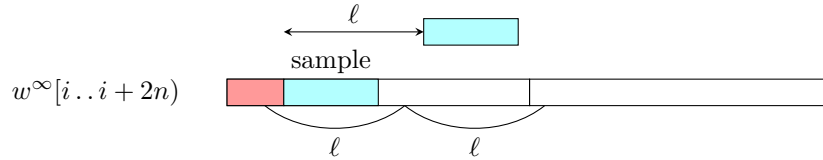
Our aim is to show that no  $\delta$ -dense words exist when  $w$  is primitive and  $\delta$  is sufficiently small.

The next lemma states that each fragment of  $\tilde{w}$  of length  $\frac{1}{2}n - \delta$  has a copy to its right at a well-specified distance  $d$ . See Figure 6 for an illustration.

► **Lemma 20** (Transporting Lemma). *Assume  $w$  is  $\delta$ -dense with positive integer  $\delta \leq \frac{1}{2}n$ . Let  $F$  be a fragment of length at most  $\frac{1}{2}n - \delta$  that occurs at some position  $i \geq n$  in  $w^\infty$ . Then,  $F$  also occurs in  $w^\infty$  at position  $i + \ell$  for some  $\ell \in (\frac{1}{2}(n - \delta) \dots \frac{1}{2}n)$ .*

**Proof.** Since  $w$  is  $\delta$ -dense, there exists a position  $j$  in  $(i - \delta \dots i]$  where a  $\delta$ -square fragment  $x = uu$  occurs in  $w^\infty$ . By the definition of a  $\delta$ -square, its total length satisfies  $n - (j - (i - \delta)) < |uu| < n$ . It follows that the half-length  $|u|$  satisfies  $\frac{1}{2}(n - \delta) < |u| < \frac{1}{2}n$ .

By Equation (2), the square  $x = uu$  ends at a position  $z \geq i - \delta + n$ , so the first half  $u$  of the square ends at a position  $z' \geq i - \delta + \frac{1}{2}n \geq i + |F|$ . Therefore the fragment  $F$  is completely contained within  $u$ . The second half of  $x$  also contains a copy of  $F$  shifted by a distance  $|u|$ . Therefore,  $F$  also occurs at position  $i + |u|$ . ◀



■ **Figure 6** Illustration of the Transporting Lemma (Lemma 20). The sample is shown in blue, and the  $\delta$ -length interval with respect to which the  $\delta$ -square occurs is shown in red.

We use the following fact from [1], whose proof relies on the periodicity lemma.

► **Fact 21** ([1, Lemma 4]). *Let  $w$  be a word and let  $a$  and  $b$  be letters. If both  $aw$  and  $wb$  are periodic, then they have the same period.*

► **Corollary 22.** *If  $w$  is primitive and  $\ell \in [1 \dots n]$ , then  $\tilde{w}$  contains a non-periodic fragment  $s$  of length  $\ell$ . We refer to this as an  $\ell$ -sample.*

**Proof.** Let us assume that  $\tilde{w}$  does not contain a non-periodic fragment of length  $\ell$ . Then, by Fact 21, all length- $\ell$  fragments of  $ww$  are periodic with the same period, i.e., the whole  $\tilde{w}$  has a period at most  $\frac{1}{2}\ell$ . By the periodicity lemma (Lemma 1),  $\tilde{w} = ww$  has a period  $p$  such that  $p \leq \frac{1}{2}n$  and  $p$  divides  $n$ . Hence,  $w$  is non-primitive. ◀

We show that, for every primitive word  $w$ ,  $\tilde{w}$  is not  $\delta$ -dense for a certain parameter  $\delta \leq 0.5n$ . Together with Lemmas 14 and 19, this implies that  $|\mathbf{S}_n(\tilde{w})| \leq 2n - \delta$ .

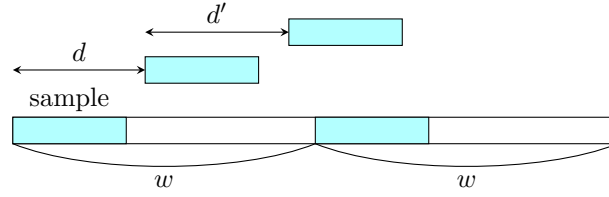


## Simple Upper Bound

First we give a simple and intuitive proof for  $\delta = \lfloor \frac{1}{6}n \rfloor$ .

► **Lemma 23.** *If  $w$  is primitive and  $n = |w| \geq 6$ , then  $\tilde{w}$  is not  $\lfloor \frac{1}{6}n \rfloor$ -dense.*

**Proof.** We prove this by contradiction. Assume that  $\tilde{w}$  is  $\lfloor \frac{1}{6}n \rfloor$ -dense. Let  $\mathbf{s}$  be a  $\lfloor \frac{1}{3}n \rfloor$ -sample that is non-periodic (as guaranteed by Corollary 22). After a suitable rotation of  $ww$ , we can assume that  $\mathbf{s}$  occurs at positions 0 and  $n$ . Due to Lemma 20,  $\mathbf{s}$  also occurs at position  $i = d + d'$ , where  $d, d' \in (\frac{1}{2} \cdot \frac{5}{6}n \dots \frac{1}{2}n)$ ; see Figure 7. Consequently,  $\mathbf{s}$  occurs at distinct positions  $n$  and  $i$  that are at distance at most  $\lfloor \frac{1}{6}n \rfloor \leq |\mathbf{s}|/2$ . Hence,  $\mathbf{s}$  is periodic, a contradiction. ◀



■ **Figure 7** Illustration of the proof of Lemma 23.

Lemmas 14, 19, and 23 imply that  $\text{CS}(n) \leq 2n - \lfloor \frac{1}{6}n \rfloor = \lceil \frac{11}{6}n \rceil$ , after a trivial verification of the cases when  $n < 6$ .

## Stronger Upper Bound

Next, we strengthen the upper bound using a more refined argument.

► **Lemma 24.** *If  $w$  is primitive, with  $n = |w| \geq 5$ , then  $\tilde{w}$  is not  $\lfloor 0.2n \rfloor$ -dense.*

**Proof.** We prove this by contradiction. Assume that  $\tilde{w}$  is  $\delta$ -dense for  $\delta = \lfloor 0.2n \rfloor$ . Let  $\mathbf{s}$  be a non-periodic sample of length  $\ell = \lfloor 0.3n \rfloor$ , (as guaranteed by Corollary 22, since  $\ell \geq 1$  for  $n \geq 4$ ). Let  $\mathbf{A}$  denote the set of starting positions of  $\mathbf{s}$  in  $ww$ .

After a suitable rotation of  $ww$ , we may assume that positions 0 and  $n$  belong to  $\mathbf{A}$ . Let  $\mathbf{A}' = \mathbf{A} \cap [0 \dots n)$ ,  $\mathbf{A}' = \{a_0, \dots, a_{|\mathbf{A}'|-1}\}$  with  $a_0 < \dots < a_{|\mathbf{A}'|-1}$  and define  $\ell_i = a_{(i+1) \bmod |\mathbf{A}'|} - a_i$  for  $i \in [0 \dots |\mathbf{A}'|)$ .

For each occurrence at position  $a_i$ , let  $d_i$  be the shift distance given by the Transporting-Lemma (Lemma 20). This lemma applies since  $\ell + \delta \leq \frac{1}{2}n$ , and it ensures that  $d_i \in (\frac{1}{2} \cdot \lceil 0.8n \rceil \dots 0.5n)$ .

Then, there exists some  $i' \in [0 \dots |\mathbf{A}'|)$  such that  $(a_i + d_i) \bmod n = a_{i'}$ . We denote  $\text{succ}(i) := i'$ , we define  $\text{succ}(i) := \text{succ}(i \bmod |\mathbf{A}'|)$ .

▷ **Claim 25.** For each  $i \in [0 \dots |\mathbf{A}'|)$ ,  $\text{succ}(\text{succ}(i)) = (i - 1) \bmod n$  and  $\ell_i \in (0.15n \dots \lfloor 0.2n \rfloor)$ .

**Proof.** Let  $\text{succ}(i) = i'$  and  $\text{succ}(i') = i''$ . The sum of two consecutive shift distances  $d_i + d_{i'} \in (\lceil 0.8n \rceil \dots n)$ . Hence,  $a_i + d_i + d_{i'} < a_i + n$ , and there is no occurrence of  $\mathbf{s}$  in  $w^\infty$  between  $a_i + d_i + d_{i'}$  and  $a_i + n$ ; otherwise,  $\mathbf{s}$  would be periodic. Therefore,  $\text{succ}(\text{succ}(i)) = (i - 1) \bmod n$ . Moreover,

$$\ell_{(i-1) \bmod n} \leq n - (\lceil 0.8n \rceil + 1) < \lfloor 0.2n \rfloor, \text{ as claimed.} \quad \triangleleft$$

▷ **Claim 26.** For each  $i \in [0 \dots |\mathbf{A}'|)$ ,  $\text{succ}(i) = (i + 3) \bmod n$ .

Proof. Each shift  $d_i$  from the Transporting-Lemma lies in  $(0.4n \dots 0.5n)$  (as  $\frac{1}{2} \cdot \lceil 0.8n \rceil \geq \frac{1}{2} \cdot 0.8n$ ), while each  $\ell_i$  lies in interval  $(0.15n \dots \lfloor 0.2n \rfloor)$  by Claim 25.

Since  $2 \cdot \lfloor 0.2n \rfloor \leq 0.4n < d_i < 0.5n < 4 \cdot 0.15n$ , each shift spans exactly three intervals. Hence,  $\text{succ}(i) = (i + 3) \bmod n$ .  $\triangleleft$

The interval bounds from Claim 25 imply that  $|\mathbf{A}'| = 6$ . But then, by Claim 26,  $\text{succ}(\text{succ}(0)) \neq |\mathbf{A}'| - 1$ , contradicting Claim 25. This completes the proof.  $\blacktriangleleft$

By Lemmas 14, 19, and 24, we obtain the upper bound  $\text{CS}(n) \leq 2n - \lfloor 0.2n \rfloor = \lceil 1.8n \rceil$ , after a trivial verification of the cases when  $n < 5$ .

► **Theorem 27.**  $\text{CS}(n) \leq \lceil 1.8n \rceil$ .

► **Remark 28.** If we used the sample size  $\lfloor 0.25n \rfloor$  as in [1], we would obtain a weaker upper bound of  $\lceil \frac{13}{7}n \rceil$ .

## 5 Limitations of our Approach

It appears that by taking larger values of  $\delta$ , one could possibly strengthen Lemma 24, showing that every primitive word is not  $\delta$ -dense, and thereby obtaining a stronger upper bound of  $2n - \delta$ . However, we show that for  $\delta = \frac{1}{3}n + 4$  this approach no longer works.

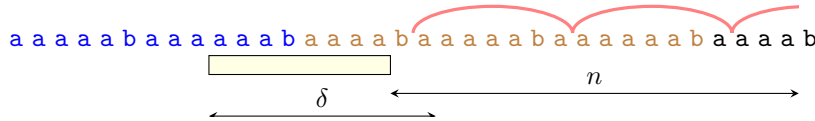
We say that a square  $uu$  kills a position  $i$  in  $w^\infty$  if  $uu$  is a  $\delta$ -square fragment with respect to the interval  $[i \dots i + \delta)$ .

► **Observation 29.**

- (a) A square  $uu$  such that  $n - (\delta - 1) < |uu| < n$  starting at position  $j$  in  $w^\infty$  kills all positions contained modulo  $n$  in the interval  $[j - (\delta - 1) \dots j + |uu| - n)$ .
- (b) For a periodic fragment  $R$  with  $n - (\delta - 1) < 2 \cdot \text{per}(R) < n$  starting at position  $j$  in  $w^\infty$ , all positions contained modulo  $n$  in the interval

$$I_R = [j - (\delta - 1) \dots j + |R| - n - 1] \quad (3)$$

are killed by the  $|R| - 2 \cdot \text{per}(R) + 1$  squares of length  $2 \cdot \text{per}(R)$  that are induced by  $R$ ; see Figure 8.



■ **Figure 8** Let  $w = a^4ba^5ba^6b$  (fragment shown in brown) and  $\delta = 10$ . The figure shows a word  $(w')^2$  for a rotation  $w'$  of  $w$ . The square fragments in  $w^\infty$  induced by the periodic fragment  $R$  (shown in red) together kill all positions contained modulo  $n$  in the interval  $I_R$  indicated by the yellow rectangle.

► **Fact 30.** There exist arbitrarily long primitive words  $w$  that are  $\delta$ -dense for  $\delta = \frac{1}{3}|w| + 4$ .

**Proof.** Let us take  $\mathcal{W}_{k,1} = a^k b a^{k+1} b a^{k+2} b$  of length  $n = 3k + 6$  and  $\delta = k + 6 = \frac{1}{3}n + 4$ . Using Equation (3), it is easy to see that each position of  $\mathcal{W}_{k,1}$  is killed by one of the following three periodic fragments:

- The fragment  $R_1 = (a^k b a)^2 a^k$  occurring at position 0 kills positions in the interval

$$[0 - (k + 5) \dots 0 + (3k + 4) - n - 1] \equiv_{\text{mod } n} [2k + 1 \dots n - 3].$$

- The fragment  $R_2 = (a^{k+1} b a)^2 a^{k-1}$  occurring at position  $k + 1$  kills positions in the interval

$$[(k + 1) - (k + 5) \dots (k + 1) + (3k + 5) - n - 1] \equiv_{\text{mod } n} [n - 4 \dots n - 1] \cup [0 \dots k - 1];$$

cf. Figure 8.

- The fragment  $R_3 = (a^k b)^2 a^k$  occurring at position  $2k + 5$  kills positions in the interval

$$[(2k + 5) - (k + 5) \dots (2k + 5) + (3k + 2) - n - 1] \equiv_{\text{mod } n} [k \dots 2k].$$

The union of the intervals  $[0 \dots k - 1]$ ,  $[k \dots 2k]$ ,  $[2k + 1 \dots n - 3]$ , and  $[n - 4 \dots n - 1]$  covers all positions in  $\mathcal{W}_{k,1}$ . This implies that every position is killed by a suitable  $\delta$ -square fragment. Hence,  $\mathcal{W}_{k,1}$  is  $\delta$ -dense.  $\blacktriangleleft$

## 6 Final Remarks

We have shown that  $1.5n - \mathcal{O}(\sqrt{n}) \leq \text{CS}(n) \leq \lceil 1.8n \rceil$ , where the lower bound holds for infinitely many  $n$ . We conjecture that the lower bound is tight, that is, that  $\text{CS}(n) \leq 1.5n$ .

Tight bounds related to repetitions and symmetries are usually non-trivial. This was, for instance, the case for bounds on standard squares (see [7, 9, 12, 5, 18, 3]) and powers ([11, 13, 14]), runs (the “runs theorem”; see [2] and references therein), and palindromes in circular words ([17]). For example, the abstract of [17] states: “*In this paper we show, with a very complicated proof, ...*”.

Possibly, the elegant graph-theoretic proof of the recent upper bound for standard squares in [3] can be adapted to establish an  $1.5n$  upper bound for distinct squares in circular words.

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