

# Finding the Largest Fixed-Density Necklace and Lyndon word

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## Abstract

We present an  $O(n)$  time algorithm for finding the lexicographically largest fixed-density necklace of length  $n$ . Then we determine whether or not a given string can be extended to a fixed-density necklace of length  $n$  in  $O(n^2)$  time. Finally, we give an  $O(n^3)$  algorithm that finds the largest fixed-density necklace of length  $n$  that is less than or equal to a given string. The efficiency of the latter algorithm is a key component to allow fixed-density necklaces to be ranked efficiently. The results are extended to find the largest fixed-density Lyndon word of length  $n$  (that is less than or equal to a given string) in  $O(n^3)$  time.

## 1 Introduction

A *necklace* is the lexicographically smallest string in an equivalence class of strings under rotation. A *Lyndon word* is a primitive (aperiodic) necklace. The *density* of a binary string is the number of 1s it contains. Let  $\mathbf{N}(n, d)$  denote the set of all binary necklaces with length  $n$  and density  $d$ . In this paper we present efficient algorithms for the following three problems:

1. finding the largest necklace in  $\mathbf{N}(n, d)$ ,
2. determining if an arbitrary string is a prefix of some necklace in  $\mathbf{N}(n, d)$ , and
3. finding the largest necklace in  $\mathbf{N}(n, d)$  that is less than or equal to a given binary string of length  $n$ .

The first problem can be answered in  $O(n)$  time, which is applied to answer the second problem in  $O(n^2)$  time, which in turn is applied to answer the third problem in  $O(n^3)$  time. The third problem can also be solved for fixed-density Lyndon words in  $O(n^3)$  time, which can immediately be used to find the largest fixed-density Lyndon word of a given length. Solving the third problem efficiently for both necklaces and Lyndon words is a key step in the first efficient algorithms to rank and unrank fixed-density necklaces and Lyndon words [2]. When there is no density constraint, the third problem is known to be solvable in  $O(n^2)$ -time; one such implementation is outlined in [10]. This problem was encountered in the first efficient algorithms to rank and unrank necklaces and Lyndon words discovered independently by Kopparty, Kumar, and Saks [5] and Kociumaka, Radoszewski and Rytter [4].

To illustrate these problems, consider the lexicographic listing of  $\mathbf{N}(8, 3)$ :

000001111, 000010111, 000011011, 000100111, 000101011, 000110011, 001001011.

The largest necklace in this set is 001001011. The string 0010 is a prefix of a necklace in this set, however, 010 is not. Given an arbitrary string  $\alpha = 00011000$ , the largest necklace in this set that is less than or equal to  $\alpha$  is 000101011.

Fixed-density necklaces were first studied by Savage and Wang when they provided the first Gray code listing in [11]. Since then, an algorithm to efficiently list fixed-density necklaces was given by Ruskey and Sawada [8] and another efficient algorithm to list them in cool-lex Gray code order was given by Sawada and

Williams [9]. The latter algorithm leads to an efficient algorithm to construct a fixed-density de Bruijn sequence by Ruskey, Sawada, and Williams [7]. When equivalence is further considered under string reversal, an algorithm for listing fixed-density bracelets is given by Karim, Alamgir and Husnine [3].

The remainder of this paper is presented as follows. In Section 2, we present some preliminary results on necklaces and related objects. In Section 3, we present an  $O(n)$ -time algorithm to find the largest necklace in  $\mathbf{N}(n, d)$ . In Section 4, we present an  $O(n^2)$ -time algorithm to determine whether or not a given string is a prefix of a necklace in  $\mathbf{N}(n, d)$ . In Section 5, we present an  $O(n^3)$ -time algorithm to finding the largest necklace in  $\mathbf{N}(n, d)$  that is less than or equal to a given string. These results on necklaces are extended to Lyndon words in Section 6.

## 2 Preliminaries

Let  $\alpha$  be a binary string and let  $lyn(\alpha)$  denote the length of the longest prefix of  $\alpha$  that is a Lyndon word. A *prenecklace* is a prefix of some necklace. The following theorem by Cattell et al. [1] has been called *The Fundamental Theorem of Necklaces*:

**Theorem 2.1** *Let  $\alpha = a_1a_2 \cdots a_{n-1}$  be a prenecklace over the alphabet  $\Sigma = \{0, 1, \dots, k-1\}$  and let  $p = lyn(\alpha)$ . Given  $b \in \Sigma$ , the string  $\alpha b$  is a prenecklace if and only if  $a_{n-p} \leq b$ . Furthermore,*

$$lyn(\alpha b) = \begin{cases} p & \text{if } b = a_{n-p} \\ n & \text{if } b > a_{n-p} \text{ (i.e., } \alpha b \text{ is a Lyndon word).} \end{cases}$$

**Corollary 2.2** *If  $\alpha b$  is a prenecklace then  $\alpha(b+1)$  is a Lyndon word.*

**Corollary 2.3** *If  $\alpha = a_1a_2 \cdots a_n$  is a necklace then  $\alpha a_1$  is a prenecklace and  $\alpha b$  is a Lyndon word for all  $b > a_1$ .*

The following is well-known property of Lyndon words by Reutenauer [6].

**Lemma 2.4** *If  $\alpha$  and  $\beta$  are Lyndon words such that  $\alpha < \beta$  then  $\alpha\beta$  is a Lyndon word.*

**Corollary 2.5** *If  $\alpha$  is a Lyndon word and  $\beta$  is a necklace such that  $\alpha \leq \beta$  then  $\alpha\beta^t$  is a necklace for  $t \geq 1$ .*

*Proof.* If  $\alpha = \beta$  then clearly  $\alpha\beta^t$  is a (periodic) necklace. If  $\beta$  is a Lyndon word, then the result follows from repeated application of Lemma 2.4. Otherwise  $\beta = \delta^i$  for some Lyndon word  $\delta$  and  $i > 1$ . Note that  $\alpha \leq \delta$  because otherwise  $\alpha > \beta$ . If  $\alpha < \delta$ , then repeated application of Lemma 2.4 implies that  $\alpha\delta^j$  is a Lyndon word for all  $j \geq 0$ . If  $\alpha = \delta$ , then clearly  $\alpha\delta^j$  is a (periodic) necklace for all  $j \geq 1$ . In both cases,  $\alpha\beta^t$  will be a necklace for all  $t \geq 1$ .  $\square$

**Lemma 2.6** *A  $k$ -ary string  $\alpha = a_1a_2 \cdots a_n$  over alphabet  $\{0, 1, \dots, k-1\}$  is a necklace if and only if  $0^{t-a_1}10^{t-a_2}1 \cdots 0^{t-a_n}1$  is a necklace for all  $t \geq k-1$ .*

*Proof.* ( $\Rightarrow$ ) Assume  $\alpha$  is a necklace. Let  $\beta = 0^{t-a_1}10^{t-a_2}1 \cdots 0^{t-a_n}1$  for some  $t \geq k-1$ . If  $\beta$  is not a necklace then there exists some  $2 \leq i \leq n$  such that  $0^{t-a_i}10^{t-a_{i+1}}1 \cdots 0^{t-a_n}10^{t-a_1}1 \cdots 0^{t-a_{i-1}}1 < \beta$ . But this implies  $a_i a_{i+1} \cdots a_n a_1 \cdots a_{i-1} < \alpha$ , contradicting the assumption that  $\alpha$  is a necklace. Thus  $\beta$  is a necklace. ( $\Leftarrow$ ) Assume  $\beta = 0^{t-a_1}10^{t-a_2}1 \cdots 0^{t-a_n}1$  is a necklace for all  $t \geq k-1$ . If  $\alpha$  is not a necklace then there exists some  $2 \leq i \leq n$  such that  $a_i a_{i+1} \cdots a_n a_1 \cdots a_{i-1} < \alpha$ . But this implies that  $0^{t-a_i}10^{t-a_{i+1}}1 \cdots 0^{t-a_n}10^{t-a_1}1 \cdots 0^{t-a_{i-1}}1 < \beta$ , contradicting the assumption that  $\beta$  is a necklace. Thus  $\alpha$  is a necklace.  $\square$

**Lemma 2.7** A  $k$ -ary string  $\alpha = a_1 a_2 \cdots a_n$  over alphabet  $\{0, 1, \dots, k-1\}$  is a necklace if and only if  $01^{t+a_1} 01^{t+a_2} \dots 01^{t+a_n}$  is a necklace for all  $t \geq 0$ .

*Proof.* ( $\Rightarrow$ ) Assume  $\alpha$  is a necklace. Let  $\beta = 01^{t+a_1} 01^{t+a_2} \dots 01^{t+a_n}$  for some  $t \geq 0$ . If  $\beta$  is not a necklace there exists some  $2 \leq i \leq n$  such that  $01^{t+a_i} 01^{t+a_{i+1}} \dots 01^{t+a_n} 01^{t+a_1} \dots 01^{t+a_{i-1}} < \beta$ . But this implies  $a_i a_{i+1} \cdots a_n a_1 \cdots a_{i-1} < \alpha$ , contradicting the assumption that  $\alpha$  is a necklace. Thus  $\beta$  is a necklace. ( $\Leftarrow$ ) Assume  $\beta = 01^{t+a_1} 01^{t+a_2} \dots 01^{t+a_n}$  is a necklace for all  $t \geq 0$ . If  $\alpha$  is not a necklace there exists some  $2 \leq i \leq n$  such that  $a_i a_{i+1} \cdots a_n a_1 \cdots a_{i-1} < \alpha$ . But this implies that  $01^{t+a_i} 01^{t+a_{i+1}} \dots 01^{t+a_n} 01^{t+a_1} \dots 01^{t+a_{i-1}} < \beta$ , contradicting the assumption that  $\beta$  is a necklace. Thus  $\alpha$  is a necklace.  $\square$

### 3 Finding the largest necklace with a given density

Let  $\text{LARGESTNECK}(n, d)$  denote the lexicographically largest binary necklace in  $\mathbf{N}(n, d)$ .

**Lemma 3.1** Let  $0 < d \leq n$  and  $t = \lfloor \frac{n}{d} \rfloor$ . Then

$$\text{LARGESTNECK}(n, d) = 0^{t-b_1} 10^{t-b_2} 1 \dots 0^{t-b_d} 1,$$

where  $b_1 b_2 \cdots b_d = \text{LARGESTNECK}(d, d - (n \bmod d))$ .

*Proof.* Since  $d > 0$ ,  $\alpha = \text{LARGESTNECK}(n, d)$  can be written as  $0^{c_1} 10^{c_2} 1 \dots 0^{c_d} 1$  where each  $c_i \geq 0$ . Let  $x = d - (n \bmod d)$ . Observe that  $\alpha \geq (0^t 1)^{d-x} (0^{t-1} 1)^x \in \mathbf{N}(n, d)$  (it is a simple calculation to verify the length). Thus,  $c_1 \leq t$ , and moreover each  $c_i \leq t$  since  $\alpha$  is a necklace. Therefore  $\alpha$  can be expressed as  $0^{t-b_1} 10^{t-b_2} 1 \dots 0^{t-b_d} 1$  for some string  $\beta = b_1 b_2 \cdots b_d$  over the alphabet  $\{0, 1, \dots, t\}$ . By Lemma 2.6,  $\beta$  is a necklace. Suppose there is some largest  $1 \leq i \leq d$  such that  $b_i > 1$ . Thus, each element of  $b_{i+1} \cdots b_d$  must be in  $\{0, 1\}$ . Since  $\beta$  is a necklace, each of its rotations  $b_j \cdots b_d b_1 \cdots b_{j-1} \geq \beta$ . Thus, we can deduce that if  $j > i$  then  $b_j \cdots b_d b_1 \cdots b_{j-1} > b_1 b_2 \cdots b_{i-1}$ . This implies that  $b_j \cdots b_d b_1 \cdots b_{i-1} > b_1 b_2 \cdots b_{i-1}$ . Now consider  $\gamma = b_1 b_2 \cdots b_{i-2} (b_{i-1} + 1) b_{i+1} \cdots b_d$ . Since  $b_1 b_2 \cdots b_{i-1}$  is a prenecklace,  $b_1 b_2 \cdots b_{i-2} (b_{i-1} + 1)$  is a Lyndon word by Corollary 2.2. Thus any proper rotation of  $\gamma$  starting before  $b_{i+1}$  will be strictly greater than  $\gamma$ . Now consider a rotation of  $\gamma$  starting from  $b_j$  for  $i+1 \leq j \leq d$ . Observe that a rotation starting from  $b_j$  has prefix  $b_j \cdots b_d b_1 \cdots b_{i-2} (b_{i-1} + 1)$ . We have already noted that  $b_j \cdots b_d b_1 \cdots b_{i-1} > b_1 b_2 \cdots b_{i-1}$ , and therefore the complete rotation of  $\gamma$  starting with  $b_j$  must be greater than  $\gamma$ . Since every proper rotation of  $\gamma$  is strictly greater than  $\gamma$ ,  $\gamma$  is a necklace. However, this means that  $\gamma(b_i - 1)$  is also a necklace by Corollary 2.3 and hence by Lemma 2.6,  $0^{b_1} 10^{b_2} 1 \dots 0^{b_{i-2}} 10^{b_{i-1}+1} 10^{b_{i+1}} 1 \dots 0^{b_d} 10^{b_i-1} 1$  is also a necklace. But this contradicts  $\alpha = \text{LARGESTNECK}(n, d)$ . Therefore there is no  $b_i > 1$  and hence  $\beta$  is a binary string. Now, since the necklace  $\beta$  is binary it must have density  $x$ . For any  $b'_1 b'_2 \cdots b'_d \in \mathbf{N}(d, x)$  we have  $\alpha' = 0^{t-b'_1} 10^{t-b'_2} 1 \dots 0^{t-b'_d} 1 \in \mathbf{N}(n, d)$  by Lemma 2.6. Clearly,  $\alpha'$  will be largest when  $b'_1 b'_2 \cdots b'_d = \text{LARGESTNECK}(d, x)$ . Thus,  $\beta = \text{LARGESTNECK}(d, x)$ .  $\square$

**Lemma 3.2** Let  $0 \leq d < n$  and  $t = \lfloor \frac{n}{n-d} \rfloor$ . Then

$$\text{LARGESTNECK}(n, d) = 01^{t-1+b_1} 01^{t-1+b_2} \dots 01^{t-1+b_{n-d}},$$

where  $b_1 b_2 \cdots b_{n-d} = \text{LARGESTNECK}(n-d, n \bmod (n-d))$ .

*Proof.* Since  $d < n$ ,  $\alpha = \text{LARGESTNECK}(n, d)$  can be written as  $01^{c_1} 01^{c_2} \dots 01^{c_{n-d}}$  where each  $c_i \geq 0$ . Let  $x = n \bmod (n-d)$ . Observe that  $\alpha \geq (01^{t-1})^{n-d-x} (01^t)^x \in \mathbf{N}(n, d)$ . Thus,  $c_1 \geq t-1$ , and moreover

each  $c_i \geq t - 1$  since  $\alpha$  is a necklace. Therefore  $\alpha$  can be expressed as  $01^{t-1+b_1}01^{t-1+b_2} \dots 01^{t-1+b_{n-d}}$  for some string  $\beta = b_1b_2 \dots b_{n-d}$  over the alphabet  $\{0, 1, \dots, d\}$ . By Lemma 2.7,  $\beta$  is a necklace. Suppose there is some largest  $1 \leq i \leq n - d$  such that  $b_i > 1$ . Thus, each element of  $b_{i+1} \dots b_{n-d}$  must be in  $\{0, 1\}$ . Since  $\beta$  is a necklace, each of its rotations  $b_j \dots b_{n-d}b_1 \dots b_{j-1} \geq \beta$ . Thus, we can deduce that if  $j > i$  then  $b_j \dots b_{n-d}b_1 \dots b_{j-1} > b_1b_2 \dots b_{i-1}$ . This implies that  $b_j \dots b_{n-d}b_1 \dots b_{i-1} > b_1b_2 \dots b_{i-1}$ . Now consider  $\gamma = b_1b_2 \dots b_{i-2}(b_{i-1}+1)b_{i+1} \dots b_{n-d}$ . Since  $b_1b_2 \dots b_{i-1}$  is a prenecklace,  $b_1b_2 \dots b_{i-2}(b_{i-1}+1)$  is a Lyndon word by Corollary 2.2. Thus any proper rotation of  $\gamma$  starting before  $b_{i+1}$  will be strictly greater than  $\gamma$ . Now consider a rotation of  $\gamma$  starting from  $b_j$  for  $i+1 \leq j \leq n-d$ . Observe that a rotation starting from  $b_j$  has prefix  $b_j \dots b_{n-d}b_1 \dots b_{i-2}(b_{i-1}+1)$ . We have already noted that  $b_j \dots b_{n-d}b_1 \dots b_{i-1} > b_1b_2 \dots b_{i-1}$ , and therefore the complete rotation of  $\gamma$  starting with  $b_j$  must be greater than  $\gamma$ . Since every proper rotation of  $\gamma$  is strictly greater than  $\gamma$ ,  $\gamma$  is a necklace. However, this means that  $\gamma(b_i - 1)$  is also a necklace by Corollary 2.3 and hence by Lemma 2.7,  $01^{b_1}01^{b_2} \dots 01^{b_{i-2}}01^{b_{i-1}+1}01^{b_{i+1}} \dots 01^{b_{n-d}}01^{b_i-1}$  is also a necklace. But this contradicts  $\alpha = \text{LARGESTNECK}(n, d)$ . Therefore there is no  $b_i > 1$  and hence  $\beta$  is a binary string. Now, since the necklace  $\beta$  is binary it must have density  $x$ . For any  $b'_1b'_2 \dots b'_{n-d} \in \mathbf{N}(n-d, x)$  we have  $\alpha' = 01^{t-1+b'_1}01^{t-1+b'_2} \dots 01^{t-1+b'_{n-d}} \in \mathbf{N}(n, d)$  by Lemma 2.7. Clearly,  $\alpha'$  will be largest when  $b'_1b'_2 \dots b'_{n-d} = \text{LARGESTNECK}(n-d, x)$ . Thus,  $\beta = \text{LARGESTNECK}(n-d, x)$ .  $\square$

By combining the previous two lemmas, the following equation can be used to recursively compute  $\text{LARGESTNECK}(n, d)$  letting  $t = \lfloor \frac{n}{d} \rfloor$  and  $s = \lfloor \frac{n}{n-d} \rfloor$ :

$$\text{LARGESTNECK}(n, d) = \begin{cases} 0^n & \text{if } d = 0 \\ 0^{t-b_1}10^{t-b_2}1 \dots 0^{t-b_d}1 & \text{if } 0 < d \leq \frac{n}{2} \\ 01^{s-1+c_1}01^{s-1+c_2} \dots 01^{s-1+c_{n-d}} & \text{if } \frac{n}{2} < d < n \\ 1^n & \text{if } d = n, \end{cases}$$

where  $b_1b_2 \dots b_d = \text{LARGESTNECK}(d, d - (n \bmod d))$  and  $c_1c_2 \dots c_{n-d} = \text{LARGESTNECK}(n-d, n \bmod (n-d))$ . Note that the strings returned in each recursive application have length less than or equal to  $\frac{n}{2}$ . Given these strings, obtaining the largest necklace can easily be constructed in  $O(n)$  time. Thus we arrive at the following theorem.

**Theorem 3.3**  $\text{LARGESTNECK}(n, d)$  can be computed in  $O(n)$  time for  $0 \leq d \leq n$ .

We conclude this section with two interesting properties of  $\text{LARGESTNECK}(n, d)$ .

**Lemma 3.4** Let  $0 \leq d \leq n$ . If  $\text{LARGESTNECK}(n, d) = a_1a_2 \dots a_n$  then  $\text{LARGESTNECK}(n, n-d) = \bar{a}_n \dots \bar{a}_2\bar{a}_1$ .

*Proof.* The proof is by induction on  $n$ . For any  $n \geq 1$ ,  $\text{LARGESTNECK}(n, 0) = 0^n$  and  $\text{LARGESTNECK}(n, n) = 1^n$ . Thus the base case when  $n = 1$  clearly holds, along with the cases when  $d = 0$  and  $d = n$ . Consider  $0 < d < n$  and let  $\text{LARGESTNECK}(n, d) = a_1a_2 \dots a_n$ . By Lemma 3.1,  $\alpha = 0^{t-b_1}10^{t-b_2}1 \dots 0^{t-b_d}1$  where  $b_1b_2 \dots b_d = \text{LARGESTNECK}(d, d - (n \bmod d))$  and  $t = \lfloor \frac{n}{d} \rfloor$ . By induction,  $\text{LARGESTNECK}(d, n \bmod d) = \bar{b}_d \dots \bar{b}_2\bar{b}_1$ . Now by applying Lemma 3.2,

$$\begin{aligned} \text{LARGESTNECK}(n, n-d) &= 01^{t-1+\bar{b}_d} \dots 01^{t-1+\bar{b}_2} \dots 01^{t-1+\bar{b}_1} \\ &= 01^{t-b_d} \dots 01^{t-b_2} \dots 01^{t-b_1} \\ &= \bar{a}_n \dots \bar{a}_2\bar{a}_1. \end{aligned}$$

$\square$

**Lemma 3.5** Let  $0 \leq d \leq n$ .  $\text{LARGESTNECK}(n, d) = \delta^j$  where  $j = \gcd(n, d)$  and  $\delta$  is some binary string of length  $\frac{n}{j}$ .

*Proof.* The proof is by induction on  $n$ . Since  $\gcd(n, 0) = \gcd(n, n) = n$ ,  $\text{LARGESTNECK}(n, 0) = 0^n$  and  $\text{LARGESTNECK}(n, n) = 1^n$ , the result clearly holds for all  $d = 0$  and  $d = n$ , and for  $n = 1$ . Suppose  $0 < d < n$  and consider  $\alpha = \text{LARGESTNECK}(n, d)$  for  $n \geq 2$ . By Lemma 3.1,  $\alpha = 0^{t-b_1}10^{t-b_2}1 \dots 0^{t-b_d}1$  where  $t = \lfloor \frac{n}{d} \rfloor$  and  $\beta = b_1b_2 \dots b_d = \text{LARGESTNECK}(d, d - n \bmod d)$ . By induction,  $\beta = \gamma^j$  where  $j = \gcd(d, d - n \bmod d)$ . Thus,  $\alpha = \delta^j$  for some  $\delta$  of length  $\frac{n}{j}$ . Finally, by applying Euclid's algorithm we have  $\gcd(n, d) = \gcd(d, n \bmod d) = \gcd(d, d - n \bmod d) = j$ .  $\square$

This final lemma implies that  $\text{LARGESTNECK}(n, d)$  is a Lyndon word if and only if  $\gcd(n, d) = 1$ .

## 4 Testing if a string is a prefix of some necklace in $\mathbf{N}(n, d)$

Let the boolean function  $\text{ISPREFIX}(\alpha, n, d)$  return True if and only if  $\alpha = a_1a_2 \dots a_t$  is a prefix of some necklace in  $\mathbf{N}(n, d)$ . In this section we present an  $O(n^2)$  implementation for this function using results from the previous section. There are two trivial conditions for the function to return true: the density constraint must be attainable and  $\alpha$  must be a prenecklace. Let  $\text{den}(\alpha)$  denote the density of  $\alpha$ . Then for the density to be attainable we must have  $0 \leq d - \text{den}(\alpha) \leq n - t$ .

Let  $\alpha = a_1a_2 \dots a_t$  be a prenecklace where  $1 \leq t \leq n$ . Let  $\text{EXTEND}(\alpha, n) = a_1a_2 \dots a_n$  be the lexicographically smallest prenecklace of length  $n$  with prefix  $\alpha$ .

**Lemma 4.1** Let  $0 \leq d \leq n$  and let  $1 \leq t \leq n$ . Suppose  $\alpha = a_1a_2 \dots a_t$  is a prenecklace and  $a_1a_2 \dots a_n = \text{EXTEND}(\alpha, n)$ . Then  $\alpha$  is a prefix of some necklace in  $\mathbf{N}(n, d)$  if and only if  $a_1a_2 \dots a_n \in \mathbf{N}(n, d)$  or there exists  $t < j \leq n$  such that  $a_j = 0$  and  $d' = d - \text{den}(a_1a_2 \dots a_{j-1}1) \geq 0$  and either:

- (1)  $j = n$  and  $d' = 0$  or
- (2)  $j < n$  and there exists  $\beta \in \mathbf{N}(n - j, d')$  such that  $a_1a_2 \dots a_{j-1}1 \leq \beta$ .

*Proof.* ( $\Rightarrow$ ) Suppose  $\alpha$  is a prefix of  $b_1b_2 \dots b_n \in \mathbf{N}(n, d)$  and suppose  $a_1a_2 \dots a_n$  is not in  $\mathbf{N}(n, d)$ . By applying Theorem 2.1, there must be some smallest  $j > t$  such that  $a_1a_2 \dots a_{j-1} = b_1b_2 \dots b_{j-1}$  with  $a_j = 0$  and  $b_j = 1$  which implies  $a_1a_2 \dots a_{j-1}1$  is a Lyndon word. Clearly  $b_{j+1}b_{j+2} \dots b_n$  has length  $n - j$  and density  $d' = d - \text{den}(a_1a_2 \dots a_{j-1}1)$ . If  $j = n$  then  $d' = 0$ . Otherwise,  $j < n$  and since  $b_1b_2 \dots b_n$  is a necklace and  $b_1b_2 \dots b_j$  is a Lyndon word, it must be that  $b_1b_2 \dots b_j \leq b_{j+1}b_{j+2} \dots b_n$ . Thus, if  $b_{j+1}b_{j+2} \dots b_n (= \beta)$  is a necklace we are done. Otherwise let  $b_{j+1}b_{j+2} \dots b_n = \delta\gamma$  such that its rotation  $\gamma\delta (= \beta)$  is a necklace. Again, since  $b_1b_2 \dots b_n$  is a necklace and  $b_1b_2 \dots b_j$  is a Lyndon word,  $b_1b_2 \dots b_j \leq \gamma$ . It follows that  $a_1a_2 \dots a_{j-1}1 = b_1b_2 \dots b_j \leq \gamma\delta$ .

( $\Leftarrow$ ) If  $a_1a_2 \dots a_n \in \mathbf{N}(n, d)$  then clearly  $\alpha$  is a prefix of some necklace in  $\mathbf{N}(n, d)$ . Otherwise, suppose there exists  $t < j \leq n$  such that  $a_j = 0$  and  $d' = d - \text{den}(a_1a_2 \dots a_{j-1}1) \geq 0$  and either (1)  $j = n$  and  $d' = 0$  or (2)  $j < n$  and there exists  $\beta \in \mathbf{N}(n - j, d')$  such that  $a_1a_2 \dots a_{j-1}1 \leq \beta$ . For either case  $a_1a_2 \dots a_{j-1}1$  is a Lyndon word since  $a_1a_2 \dots a_j$  is a prenecklace. Thus, if  $j = n$  and  $d' = 0$ , then  $a_1a_2 \dots a_{n-1}1$  is a necklace with density  $d$ . Otherwise,  $a_1a_2 \dots a_{j-1}1\beta$  is a binary string of length  $n$  and density  $d$ . By Corollary 2.5  $a_1a_2 \dots a_{j-1}1\beta$  is a necklace. Thus  $\alpha$  is a prefix of some necklace in  $\mathbf{N}(n, d)$ .  $\square$

Assuming the density constraints are attainable, and  $\alpha = a_1a_2 \dots a_t$  is a prenecklace, we can directly apply Lemma 4.1 to determine  $\text{ISPREFIX}(\alpha, n, d)$ . To apply this lemma, note that it suffices only to compare  $\beta = \text{LARGESTNECK}(n - j, d - \text{den}(a_1a_2 \dots a_{j-1}1))$  to  $a_1a_2 \dots a_{j-1}1$ , for a given  $j$ . Repeated applications

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**Algorithm 1** Testing if  $\alpha = a_1a_2 \cdots a_t$  is a prefix of a necklace in  $\mathbf{N}(n, d)$ .

---

```

1: function ISPREFIX( $\alpha, n, d$ ) returns boolean
2:   if ( $d < \text{den}(\alpha)$  or  $d - \text{den}(\alpha) > n - t$ ) then return False
3:   if  $\alpha$  is not a prenecklace then return False
4:    $a_1a_2 \cdots a_n \leftarrow \text{EXTEND}(\alpha)$ 
5:   if  $a_1a_2 \cdots a_n \in \mathbf{N}(n, d)$  then return True
6:   for  $j \leftarrow t + 1$  to  $n$  do
7:      $d' = d - \text{den}(a_1a_2 \cdots a_{j-1}1)$ 
8:     if  $a_j = 0$  and  $d' \geq 0$  then
9:       if  $j = n$  and  $d' = 0$  then return True
10:    if  $j < n$  and  $a_1a_2 \cdots a_{j-1}1 \leq \text{LARGESTNECK}(n - j, d')$  then return True
11:  return False

```

---

of Theorem 2.1 can be used to test if  $\alpha$  is a prenecklace and to compute  $\text{EXTEND}(\alpha, n)$  in  $O(n)$  time. Pseudocode for  $\text{ISPREFIX}(\alpha, n, d)$  is given in Algorithm 1.

Since  $\text{LARGESTNECK}(n, d)$  can be computed in  $O(n)$  time, we obtain the following theorem.

**Theorem 4.2**  $\text{ISPREFIX}(\alpha, n, d)$  can be computed in  $O(n^2)$  time for  $0 \leq d \leq n$ .

## 5 The largest necklace that is less than or equal to a given string

Let  $\text{LN}(\alpha, n, d)$  be a function that returns the largest necklace in  $\mathbf{N}(n, d)$  that is less than or equal to a given binary string  $\alpha = a_1a_2 \cdots a_n$ , or  $\epsilon$  (the empty string) if no such necklace exists. In this section we present an  $O(n^3)$  implementation of this function by applying the results from the previous section.

Let  $\beta = \text{LN}(\alpha, n, d)$ . If  $\alpha \in \mathbf{N}(n, d)$  then clearly  $\beta = \alpha$ . Otherwise, let  $t > 0$  be the largest index such that  $a_t = 1$  and  $a_1a_2 \cdots a_{t-1}0$  is a prefix of some necklace in  $\mathbf{N}(n, d)$ . If no such index  $t$  exists, then there is no necklace in  $\mathbf{N}(n, d)$  that is less than  $\alpha$  and thus  $\beta = \epsilon$ . If  $t$  exists, then since it was chosen to be the largest index satisfying the conditions,  $a_1a_2 \cdots a_{t-1}0$  will be the first  $t$  characters of  $\beta = b_1b_2 \cdots b_n$ . The next character  $b_{t+1}$  will be the largest element so  $b_1b_2 \cdots b_{t+1}$  is a prefix of some necklace in  $\mathbf{N}(n, d)$ . This can be determined by calling  $\text{ISPREFIX}(b_1b_2 \cdots b_t1, n, d)$ ; if it returns true, then  $b_{t+1} = 1$  and otherwise  $b_{t+1} = 0$ . The remaining characters  $b_{t+2}, b_{t+3}, \dots, b_n$  can be computed in the same way. Pseudocode for  $\text{LN}(a_1a_2 \cdots a_n, n, d)$  is given in Algorithm 2.

---

**Algorithm 2** Computing the largest necklace less than or equal to a given string.

---

```

1: function LN( $\alpha, n, d$ ) returns necklace
2:   if  $\alpha \in \mathbf{N}(n, d)$  then return  $\alpha$ 
3:    $t \leftarrow n$ 
4:   while  $t > 0$  and not ( $a_t = 1$  and  $\text{ISPREFIX}(a_1a_2 \cdots a_{t-1}0, n, d)$ ) do  $t \leftarrow t - 1$ 
5:   if  $t = 0$  then return  $\epsilon$ 
6:    $b_1b_2 \cdots b_t \leftarrow a_1a_2 \cdots a_{t-1}0$ 
7:   for  $j \leftarrow t + 1$  to  $n$  do
8:     if  $\text{ISPREFIX}(b_1b_2 \cdots b_{j-1}1, n, d)$  then  $b_j \leftarrow 1$ 
9:     else  $b_j \leftarrow 0$ 
10:  return  $b_1b_2 \cdots b_n$ 

```

---

Since  $\text{ISPREFIX}(\alpha, n, d)$  can be computed in  $O(n^2)$  time, we obtain the following theorem.

**Theorem 5.1**  $\text{LN}(\alpha, n, d)$  can be computed in  $O(n^3)$  time for  $0 \leq d \leq n$ .

## 6 Lyndon words

In this final section, we extend the results for necklaces to Lyndon words.

**Lemma 6.1** *Let  $\alpha, \beta$  be two consecutive necklaces in the lexicographic ordering of  $\mathbf{N}(n, d)$ . Then at least one of  $\alpha$  and  $\beta$  is a Lyndon word.*

*Proof.* Suppose  $\alpha < \beta$ . If  $\alpha$  is a Lyndon word we are done. Otherwise,  $\alpha = \gamma^i$  for some Lyndon word  $\gamma = a_1 a_2 \cdots a_{\frac{n}{i}}$  with density  $\frac{d}{i}$  where  $i \geq 2$ . Let  $\delta = \text{LARGESTNECK}(\frac{n}{i}, \frac{d}{i})$ . Suppose  $\gamma = \delta$ . By Lemma 3.5,  $\text{LARGESTNECK}(n, d) = \sigma^j$  where  $j = \gcd(n, d)$  and  $\sigma$  has length  $\frac{n}{j}$ . Since  $i$  divides both  $n$  and  $d$ ,  $i$  also divides  $j$ . By the definitions of  $\delta$  and  $\sigma$ ,  $\delta = \sigma^{\frac{j}{i}}$ , and thus  $\alpha = \text{LARGESTNECK}(n, d)$ . But this contradicts that  $\alpha < \beta$ . Thus,  $\gamma \neq \delta$ . Repeated application of Lemma 2.4 implies that  $\gamma^{i-1}\delta$  is a Lyndon word that is greater than  $\alpha$ . Thus the necklace  $\beta$  must have prefix  $\gamma^{i-1}$  and hence clearly is a Lyndon word.  $\square$

The following two-step algorithm will return the largest Lyndon word with length  $n$  and density  $d > 0$  that is less than or equal to  $\alpha$ , or  $\epsilon$  if no such Lyndon word exists. Let  $\beta = \text{LN}(\alpha, n, d)$ . If  $\beta$  is a Lyndon word or  $\epsilon$ , then return  $\beta$ . Otherwise  $\beta = b_1 b_2 \cdots b_n$  is a necklace where  $b_n = 1$  since  $d > 0$ . Thus,  $b_1 b_2 \cdots b_{n-1} 0$  is the largest string less than  $\beta$  and hence  $\gamma = \text{LN}(b_1 b_2 \cdots b_{n-1} 0, n, d)$  will give the second largest necklace that is less than or equal to  $\alpha$  or  $\epsilon$  if no such necklace exists. Thus the algorithm returns  $\gamma$  as either  $\gamma = \epsilon$  (no such Lyndon word exists), or by Lemma 6.1,  $\gamma$  is a Lyndon word.

Since testing whether or not a string is a Lyndon word can easily be tested in  $O(n)$  time by applying Theorem 2.1, the running time of this algorithm will be  $O(n^3)$ .

**Lemma 6.2** *The largest Lyndon word of length  $n$  and density  $d$  that is less than or equal to  $\alpha = a_1 a_2 \cdots a_n$  can be computed in  $O(n^3)$  time for  $0 < d < n$ .*

Setting  $\alpha = 1^n$ , the previous lemma immediately implies the following result.

**Corollary 6.3** *The largest Lyndon word of length  $n$  and density  $d$  can be computed in  $O(n^3)$  time for  $0 < d < n$ .*

Finally, the following conjecture has been verified to be true for all  $n < 600$  by applying the algorithm just described.

**Conjecture 6.4** *Let  $\alpha = a_1 a_2 \cdots a_n = \text{LARGESTNECK}(n, d)$  where  $p = \text{lyn}(\alpha)$  for  $0 < d < n$ . If  $p = n$ , then the largest Lyndon word of length  $n$  and density  $d$  is  $\alpha$ ; otherwise it is  $a_1 a_2 \cdots a_{p-1} 0 a_2 \cdots a_p (a_1 a_2 \cdots a_p)^{\frac{n}{p}-2}$ .*

A proof of this conjecture implies that the largest Lyndon word of length  $n$  and density  $d$  can be computed in  $O(n)$  time for  $0 < d < n$ .

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