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Minimum pattern length for short spaced seeds based on linear rulers (revised)

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Minimum pattern length for short spaced seeds based on linear rulers (revised)

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Abstract. We study the minimum pattern length for spaced seeds of the form $\mathbf{0}^{s_0} R_d \mathbf{0}^{s_1}$, with R_d a complete d-ruler and $\max(s_0, s_1) \leq d$. We show how such minimum pattern length depends on the positions in which the integers $\leq d$ are measured inside the ruler R_d.

1 Introduction

In this manuscript we analyze in detail the minimum pattern length of spaced seeds of the shape $\mathbf{0}^{s_0} R_d \mathbf{0}^{s_1}$, with R_d a complete linear d-ruler and $\max(s_0, s_1) \leq d$. We show that these bounds depend heavily on the structure of the string R_d.

The results of this manuscript are a complement to the results in [1] to which the reader should refer for motivations and background.

2 Definitions and known results

The notion of *perfect ruler*, has been studied by mathematicians for more than sixty years [2, 4, 6] (in earlier works rulers were called *difference bases*). Here we recall the basic definitions using modern terminology [5]. We base the definition of rulers on the concept of *measure*:

Definition 1 (Measure). *Let U be a binary string. For any positive integer δ we say that U* measures *δ if there exist i, j, $0 \leq i < j < |U|$, such that $j - i = \delta$ and $U[i] = U[j] = \mathbf{1}$. The pair (i, j) is said to be a* measure *of δ in U.* □

Definition 2 (Complete ruler). *Let R be a binary string of length $d+1$ such that $R[0] = \mathbf{1}$, $R[d] = \mathbf{1}$, and such that for any integer $\delta, 0 \leq \delta \leq d$, R measures δ. The string R is said to be a* complete d-ruler*, or simply a* complete ruler *when the length of R is clear from the context.* □

Intuitively, using the **1**'s as marks, with a complete d-ruler we can measure all distances between 1 and d. For example, the string **110101** is a complete 5-ruler. Note that even the string $\mathbf{1}^6 =$ **111111** is a complete 5-ruler, but not an interesting one: the challenge of rule design is to find complete d-rulers with as few marks as possible. This notion is captured by the following definition.

Definition 3 (Perfect ruler). *Let R be a complete d-ruler containing ℓ $\mathbf{1}$'s. If there exists no complete d-ruler with less than ℓ $\mathbf{1}$'s then R is said to be a* perfect d-ruler. □

Tables of all perfect rulers of size up to 101 are available on the net [5].

The structure of complete rulers naturally suggests their use for the design of spaced seeds. Given a d-ruler R, if we replace each $\mathbf{0}$ with a '#' symbol and each $\mathbf{1}$ with a '-' symbol we obtain a seed in which there is a pair of don't care symbols at distance δ for $\delta = 1, \ldots, d$. This seed solves the $(m, 2)$-problem for $m \geq 2d + 1$. However, this is not the only seed we can derive from R. For any pair s_0, s_1 the seed derived from the string $\mathbf{0}^{s_0} R \mathbf{0}^{s_1}$ also has pairs of don't care symbols at distance δ for $\delta = 1, \ldots, d$. Hence, it solves the $(m, 2)$-problem for a sufficiently large m. Clearly there is a trade-off here: the larger are s_0 and s_1 the higher is the weight of the corresponding seed (a good thing) and the larger is the value m for which the seed solves the $(m, 2)$-problem (a bad thing).

To evaluate to what extent rulers are useful for seed design it is clearly necessary to investigate this trade-off. In this section we give upper bounds to the minimum m for which the seed associated to the string $\mathbf{0}^{s_0} R \mathbf{0}^{s_1}$ solves the $(m, 2)$-problem. The results of this section are valid for any complete d-ruler R.

Since the main object of our study are rulers, for simplicity we will only work with strings over the alphabet $\{\mathbf{0}, \mathbf{1}\}$, with the *implicit* associations[1] $\mathbf{0} \to$ #, $\mathbf{1} \to$ -. We introduce Definition 4 and Lemma 1 that essentially restate known properties of seeds in the language of strings over the alphabet $\{\mathbf{0}, \mathbf{1}\}$. In the following we state these properties for any k, even if in this manuscript we are only concerned with the case

Definition 4 (Completeness). *A binary string P is (m, k)-complete if, for any length-m binary string V containing exactly k $\mathbf{1}$'s, there exists at least an index t, with $0 \leq t \leq |V| - |P|$, such that for $i = 0, \ldots, |V| - 1$, it is*

$$V[i] = \mathbf{1} \quad \Longrightarrow \quad (i - t < 0) \ \vee \ (i - t \geq |P|) \ \vee \ (P[i - t] = \mathbf{1}). \tag{1}$$

If (1) holds we say that $P + t$ matches in V, or that P shifted by t matches in V. □

Note that $P + t$ matches in V if the $\mathbf{1}$'s in V are either outside $P + t$ or correspond to a $\mathbf{1}$ in $P + t$. Equivalently, there is no $\mathbf{1}$ in V corresponding to a $\mathbf{0}$ in $P + t$.

Lemma 1. *The binary string P is (m, k)-complete if and only if the spaced seed obtained with the map $\mathbf{0} \to$ #, $\mathbf{1} \to$ - solves the (m, k)-problem.* □

Having stated Lemma 1, in the rest of this manuscript most of the results will simply establish that certain binary strings are, or are not, (m, k)-complete, without even mentioning the immediate consequence that the corresponding seeds solve, or do not solve, the (m, k)-problem.

[1] Unfortunately, this is the opposite of [3], where $\mathbf{0}$ corresponds to a don't care symbol.

Definition 5 (Minimum pattern length m_P^*). *Given a binary string P we denote by m_P^* the smallest integer m such that P is $(m, 2)$-complete.*[2] □

In [1] it is proven the following upper bound on the minimum pattern length for a seed P obtained from a d-ruler R_d.

Theorem 1 (see [1]). *Let $P = \mathbf{0}^{s_0} R \mathbf{0}^{s_1}$ where R is a complete d-ruler. If $\max(s_0, s_1) \leq d$, then $m_P^* \leq 2|P| - 1 - \min(s_0, s_1)$.*

We introduce a specific notation for the upper bound of Theorem 1, for future reference:

Definition 6 (Upper bound m_P). *For any string $P = \mathbf{0}^{s_0} U \mathbf{0}^{s_1}$, we denote by m_P the value $m_P = 2|P| - 1 - \min(s_0, s_1)$.* □

The above upper bound is valid for any d-ruler R_d. In this paper we address the question of whether this upper bound is tight.

3 Analysis of the minimum pattern length

Table 1 shows that the upper bound of Theorem 1 is not always tight. In Table 1 we compare it with the actual minimum pattern length for patterns $P = \mathbf{0}^s R_d \mathbf{0}^s$, for some values of d and some $s \leq d$. These values of the minimum pattern length are computed by direct inspection. The first column in the table gives the value of d, the second specifies the ruler for which the minimum pattern length is computed, the third column gives the value of s, the fourth reports the upper bound m_P from Theorem 1, the fifth gives the minimum pattern length m_P^*, and the last one gives the difference $m_P - m_P^*$ for quick reference. In the table we only report m_P^* for the values of $s \leq d$ for which $m_P^* < m_P$. For values of $s \leq d$ larger than those reported for each d, $m_P^* = m_P$.

In view of the values of m_P^* in Table 1, it is interesting to establish in which cases the upper bound m_P is tight, and whether there are seeds of the form $P = \mathbf{0}^{s_0} R_d \mathbf{0}^{s_1}$ for which m_P^* is significantly smaller than m_P. In [1] lower bounds for m_P^* are established on the basis on a property of the ruler R_d called its skewness, which is based on the positions of measures of integers δ in R_d.

In the next section we prove an exact relation between the positions of **1**'s in a ruler and the minimum pattern length for the derived seed.

We need an extended notion of measure of a given integer δ. We will consider, along with proper measures of δ also additional ordered pairs $(a, a + \delta)$ that have one or even both endpoints ouside of P. We will then show that the maximum distance, taken over all δ's, between two consecutive "measures" (in this extended sense) of a δ, determines the minimum pattern length.

[2] m_P^* also depends on k, but since in this manuscript we treat uniquely the case $k = 2$, k does not appear in m_P^* to make the notation less cumbersome.

d	R_d	s	m_P	m_P^*	$m_P - m_P^*$
6	**1100101**	0	13	12	1
11	**110000110101**	0	23	21	2
		1	26	23	3
		2	29	27	2
		3	32	30	2
12	**1100000110101**	0	25	23	2
		1	28	25	3
		2	31	29	2
		3	34	32	2
13	**11100010001001**	0	27	26	1
		1	30	29	1
14	**110001001010101**	0	29	28	1
15	**1100000011010101**	0	31	29	2
		1	34	31	3
		2	37	33	4
		3	40	36	4
		4	43	41	2
		5	46	44	2
16	**11000000011010101**	0	33	31	2
		1	36	33	3
		2	39	35	4
		3	42	38	4
		4	45	43	2
		5	48	46	2
17	**110000001001010101**	0	35	34	1

Table 1. A comparison of the upper bound m_P from Theorem 1 and of the actual minimum pattern length m_P^*, computed by direct inspection, for $P = \mathbf{0}^s R_d \mathbf{0}^s$, for some values of d and $s \leq d$.

Definition 7 (Maximum gap). *Let P be any spaced seed. We use the convention that $P[j] = \mathbf{1}$ for any $j < 0$ and $j \geq |P|$. For any $1 \leq \delta \leq |P|$, let $0 < a_1 < a_2 < \cdots < a_k \leq |P|$ be all the integers $0 < j \leq |P|$ such that $P[j] = P[j + \delta] = \mathbf{1}$. In addition, let a_0 denote the largest $j \leq 0$ such that $P[j] = P[j + \delta] = \mathbf{1}$.*

We define the maximum gap Γ_δ as the largest distance between consecutive a_i's, that is, $\Gamma_\delta = \max_{1 \leq j \leq k}(a_j - a_{j-1})$. □

The convention adopted in the definition is consistent with the use of spaced seeds: whether P matches in V does not change if we add to P leading or trailing **1**s (provided that V is long enough). Notice that it is always $a_k = |P|$, because we agreed that $P[j] = \mathbf{1}$ for $j \geq |P|$. Also, a_0 always exists and $-\delta - 1 \leq a_0 \leq 0$. It achieves its minimum value when $P[j] = \mathbf{0}$ for all j, $j = 0, \ldots, \delta$; it is $a_0 = 0$ when $P[0] = P[\delta] = \mathbf{1}$; otherwise it is the maximum value $a_0 < 0$ such that $a_0 + \delta \geq 0$ and $P[a_0 + \delta] = \mathbf{1}$. Since both a_0 and a_k always exist, Γ_δ is well defined.

Theorem 2. *Let P be any binary string. Let Γ_δ be defined for each $1 \leq \delta \leq |P|$ as in Definition 7. Then, the minimum m such that P is $(m, 2)$-complete is*

$$m_P^* = |P| + \max_{1 \leq \delta \leq |P|} \Gamma_\delta - 1.$$

Proof. We first prove that P is $(m_P^*, 2)$-complete. Let V be a binary string of length m_P^* and with two $\mathbf{1}$'s in the positions v_1 and v_2. Let $\delta = v_2 - v_1$. If $\delta > |P|$ we have that $P + t$ matches in V for $t = v_1 + 1$.

If $\delta \leq |P|$, let $\{a_i | i = 0, \ldots, k\}$ denote the starting points of the measures of δ defined as in Definition 7. If $v_1 = a_i$ for some $0 \leq i \leq k$, then each v_i is either outside P or $P[v_i] = \mathbf{1}$, by definition of the a_i's. Then P matches in V. If $v_1 > a_k = |P|$ then also $v_2 > |P|$, and P matches in V. Finally, if there exists a_i, with $i < k$, such that $a_i < v_1 < a_{i+1}$ we have that $P + t$ matches in V for $t = v_1 - a_i$. Since $|V| = |P| + \max_{1 \leq \delta \leq |P|} \Gamma_\delta - 1$, and $t \leq a_{i+1} - a_i - 1 \leq \Gamma_\delta - 1$, then $t \leq |V| - |P|$ so t is admissible.

In order to prove minimality, let δ' be such that $m_P^* = |P| + \Gamma_{\delta'} - 1$. let $\{a_i | i = 0, \ldots, k\}$ denote the starting points of the measures of δ' defined as in Definition 7. Let j be such that $a_{j+1} - a_j = \Gamma_{\delta'}$.

Consider the binary string V of length $m_P^* - 1 = |P| + \Gamma_{\delta'} - 2$, with exactly two $\mathbf{1}$'s, in positions $v_1 = a_{j+1} - 1$ and $v_2 = v_1 + \delta'$. By construction, the minimum value of t for which $P + t$ matches in V would be $t = a_{j+1} - a_j - 1 = \Gamma_{\delta'} - 1$. But since $|V| = |P| + \Gamma_{\delta'} - 2$, such value of t is not admissible, and therefore P is not $(m_P^* - 1, 2)$-complete. □

Theorem 2 gives an insight on the positions of $\mathbf{1}$'s in seeds that have specific completeness properties. We first notice how it implies that the bounds on s_0 and s_1 are necessary in Theorem 1:

Corollary 1. *Let $P = \mathbf{0}^{s_0} R_d \mathbf{0}^{s_1}$, with R_d a complete d-ruler. If $\min(s_0, s_1) > d$, then $m_P^* \geq 2|P| + \min(s_0, s_1)$. If, on the other hand, $\min(s_0, s_1) \leq d$ but $max(s_0, s_1) > d$, then $m_P^* \geq 2|P|$.*

Proof. Without loss of generality, let $s_0 \geq s_1$.

If both $s_0 \geq s_1 > d$, then consider a_0 and a_1 defined as in Definition 7 for $\delta = s_1$; since $\delta > d$ there are no measures of δ inside P, and $a_0 = -s_1 - 1$ and $a_1 = |P|$. Then, $\Gamma_{s_1} \geq a_1 - a_0 = |P| + s_1 + 1$ and, by Theorem 2, $m_P^* \geq 2|P| + s_1 = 2|P| + \min(s_0, s_1)$ as claimed.

On the other hand, if $s_0 > d \geq s_1$, then a_0 and a_1 defined according Definition 7 for $\delta = d + 1$ are $a_0 = -d - 2$ and $a_1 = s_0 + d$ (and $a_2 = a_k = |P|$). Then, $\Gamma_d \geq a_1 - a_0 = s_0 + 2d + 2$. Therefore, $m_P^* \geq |P| + s_0 + 2d + 1 \geq 2|P|$, since $s_1 \leq d$. □

As another consequence of Theorem 2, we show that the upper bound m_P is tight for $P = \mathbf{0}^d R_d \mathbf{0}^d$:

Corollary 2. *Let $P = \mathbf{0}^d R_d \mathbf{0}^d$, with R_d a complete d-ruler. Then $m_P^* = m_P$.*

Proof. In the hypotheses given, a_0 and a_1 for $\delta = d$ are $a_0 = -d-1$ and $a_1 = d$. Then, $\Gamma_d \geq a_1 - a_0 = 2d+1$ and, by Theorem 2, $m_P^* \geq |P| + 2d$. The thesis follows since by Theorem 1 it is $m_P^* \leq 2|P| - 1 - d = |P| + 2d$. □

The next result shows that the upper bound of Theorem 1 is tight also if a small integer has a unique measure in R_d, which is at one endpoint of R_d:

Corollary 3. *Let $P = \mathbf{0}^{s_0} R_d \mathbf{0}^{s_1}$, with R_d a complete d-ruler.*

If $s_1 = \min(s_0, s_1)$ and there exists $\delta \leq s_0$ that has in R_d the unique measure $(d-\delta, d)$, then $m_P^* = m_P$.

If $s_0 = \min(s_0, s_1)$, and there exists $\delta \leq s_1$ that has in R_d the unique measure $(0, \delta)$, then $m_P^* = m_P$.

Proof. Let $s_1 = \min(s_0, s_1)$, and δ have in R_d the unique measure $(d-\delta, d)$. Applying Definition 7 to δ, it is $a_0 = -\delta - 1$ and $a_1 = s_0 + d - \delta$. Then, $\Gamma_\delta \geq a_1 - a_0 = s_0 + d + 1$ and, by Theorem 2, $m_P^* \geq |P| + s_0 + d = 2|P| - 1 - \min(s_0, s_1) = m_P$.

Similarly, if $s_0 = \min(s_0, s_1)$ and the unique measure of a $\delta \leq s_1$ is $(0, \delta)$, applying Definition 7 to δ, it is $a_1 = s_0$ and $a_2 = |P|$. Then, $\Gamma_\delta \geq |P| - s_0$ and, by Theorem 2, $m_P^* \geq 2|P| - s_0 - 1 = 2|P| - 1 - \min(s_0, s_1) = m_P$. □

In view of these results, let us analyze some of the data from Table 1.

Example 1. As remarked above, in Table 1, we only listed for each ruler those values of s for which $m_P^* < m_P$. This means that for the specific d-rulers listed for $d = 6$, $d = 14$ and $d = 17$, it is $m_P^* = m_P$ already for $s_0 = s_1 = 1$. Indeed notice that in these three rulers $\delta = 1$ has only one measure at the very beginning of the ruler. Therefore, by Corollary 3, for $s_1 \geq 1$, $m_P^* = m_P$. In all other rulers listed in Table 1, the value $\delta = 1$ has more than one measure. □

Example 2. The 13-ruler of Table 1 has a unique measure for $\delta = 2$ in $(0, 2)$. Accordingly, by Corollary 3, it is $m_P^* = m_P$ for $s_1 \geq 2$. □

Example 3. Consider the 11-ruler $R_{11} = \mathbf{110000110101}$. The smallest integer that has a unique measure at one endpoint of R_{11} is $\delta = 4$, whose measure is $(7, 11)$.

For $s_0 = s_1 = 0$ and $\delta = 4$, the values of a_i as by Definition 7, are $a_0 = -3$, $a_1 = 7$, $a_2 = 9$, $a_3 = 11$ and $a_4 = 12$. Then, $\Gamma_4 \geq 10$ and $m_P^* \geq |P| + \Gamma_4 - 1 \geq 21$. It can be checked by direct inspection that indeed $\Gamma_4 = \max_{1 \leq \delta \leq |P|+1} \Gamma_\delta$.

For $s_0 = s_1 = 1$, Γ_4 is again the maximum among all Γ_δ's and $\Gamma_4 = a_1 - a_0 = 10$ since $a_0 = -2$, $a_1 = 8$, $a_2 = 10$, $a_3 = 12$ and $a_4 = 14$. Here $|P| = 14$ and thus $m_P^* = 23$.

For $s_0 = s_1 = 2$, $\Gamma_4 = 10$ once again, but this time it is not the maximal Γ_δ. The reason is that, with two leading zeroes, the values a_i for $\delta = 2$ are now further apart: $a_0 = -3$, $a_1 = 9$, $a_2 = 11$ and $a_3 = 16$. Therefore, $\Gamma_2 = 12$, and since $|P| = 16$, $m_P^* = 27$. Yet, since 2 has two measures, again Corollary 3 does not apply.

For $s_0 = s_1 = 3$, the argument is similar as for $s_0 = s_1 = 2$: $\Gamma_4 = \Gamma_2 = 13$ are maximal, but not large enough to have $m_P^* = m_P$, because 4 is still larger than s_0 and 2 has two measures.

Finally, for $s_0, s_1 \geq 4$, by Corollary 3, $m_P^* = m_P$. Indeed, for $s_0 = s_1 = 4$, $\delta = 4$ is now smaller than s_0 and has a unique measure at the end of R_{11}. Now $a_0 = -5$, $a_1 = 11$ and $a_2 = |P| = 17$, so $\Gamma_4 = 16$. Notice that in this case $a_1 - a_0 = s_0 + d$. □

References

1. Lavinia Egidi and Giovanni Manzini. Spaced seeds design using perfect rulers. In Roberto Grossi, Fabrizio Sebastiani, and Fabrizio Silvestri, editors, *SPIRE*, volume 7024 of *Lecture Notes in Computer Science*, pages 32–43. Springer, 2011.
2. P. Erdós and I. S. Gál. On the representation of $1, 2, \ldots, n$ by differences. *Indagationes Math.*, 10:379–382, 1948.
3. Martin Farach-Colton, Gad M. Landau, Süleyman Cenk Sahinalp, and Dekel Tsur. Optimal spaced seeds for faster approximate string matching. *J. Comput. Syst. Sci.*, 73(7):1035–1044, 2007.
4. J. Leech. On the representation of $1, 2, \ldots, n$ by differences. *J. London Math. Soc.*, 31:160–169, 1956.
5. Peter Luschny. Perfect and optimal rulers, 2003. http://www.luschny.de/math/rulers/prulers.html.
6. B. Wichmann. A note on restricted difference bases. *J. London Math. Soc.*, 38:465–466, 1962.