# Motif matching using gapped patterns\*

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Abstract. We present new algorithms for the problem of *multiple string* matching of gapped patterns, where a gapped pattern is a sequence of strings such that there is a gap of fixed length between each two consecutive strings. The problem has applications in the discovery of transcription factor binding sites in DNA sequences when using generalized versions of the Position Weight Matrix model to describe transcription factor specificities. In these models a motif can be matched as a set of gapped patterns with unit-length keywords. The existing algorithms for matching a set of gapped patterns are worst-case efficient but not practical, or vice versa, in this particular case. The novel algorithms that we present are based on dynamic programming and bit-parallelism, and lie in a middle-ground among the existing algorithms. In fact, their time complexity is close to the best existing bound and, yet, they are also practical. We also provide experimental results which show that the presented algorithms are fast in practice, and preferable if all the strings in the patterns have unit-length.

### 1 Introduction

We consider the problem of matching a set  $\mathcal{P}$  of gapped patterns against a given text of length n, where a gapped pattern is a sequence of strings, over a finite alphabet  $\Sigma$  of size  $\sigma$ , such that there is a gap of fixed length between each two consecutive strings. We are interested in computing the list of matching patterns for each position in the text. This problem is a specific instance of the Variable Length Gaps problem [3] (VLG problem) for multiple patterns and has applications in the discovery of transcription factor (TF) binding sites in DNA sequences when using generalized versions of the Position Weight Matrix (PWM) model to represent TF binding specificities. The paper [8] describes how a motif represented as a generalized PWM can be matched as a set of gapped patterns with unit-length keywords, and presents algorithms for the restricted case of patterns with two unit-length keywords.

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In the VLG problem a pattern is a concatenation of strings and of variablelength gaps. An efficient approach to solve the problem for a single pattern is based on the simulation of nondeterministic finite automata [12,6]. A method to solve the case of one or more patterns is to translate the patterns into a regular expression [13,4]. The best time bound for a regular expression is  $O(n(k \frac{\log w}{w} +$  $\log \sigma$ ) [4], where k is the number of the strings and gaps in the pattern and w is the machine word size in bits. Observe that in the case of unit-length keywords  $k = \Theta(\operatorname{len}(\mathcal{P}))$ , where  $\operatorname{len}(\mathcal{P})$  is the total number of alphabet symbols in the patterns. There are also algorithms efficient in terms of the total number  $\alpha$  of occurrences of the strings in the patterns (keywords) within the text  $[10,15,3]^{5}$ . The best bound obtained for a single pattern is  $O(n \log \sigma + \alpha)$  [3]. This method can also be extended to multiple patterns. However, if all the keywords have unit length this result is not ideal, because in this case  $\alpha$  is  $\Omega(n\frac{\operatorname{len}(\mathcal{P})}{\sigma})$  on average if we assume that the symbols in the patterns are sampled from  $\Sigma$  according to a uniform distribution. A similar approach for multiple patterns [9] leads to  $O(n(\log \sigma + K) + \alpha')$  time, where K is the maximum number of suffixes of a keyword that are also keywords and  $\alpha'$  is the number of text occurrences of pattern prefixes that end with a keyword. This result may be preferable in general when  $\alpha' < \alpha$ . In the case of unit-length keywords, however, a lower bound similar to the one on  $\alpha$  holds also for  $\alpha'$ , as the prefixes of unit length have on average  $\Omega(n\frac{|\mathcal{P}|}{\sigma})$  occurrences in the text. Recently, a variant of this algorithm based on word-level parallelism was presented in [18]. This algorithm works in time  $O(n(\log \sigma + (\log |\mathcal{P}| + \frac{k}{w})\alpha_m))$ , where k in this case is the maximum number of keywords in a single pattern and  $\alpha_m \geq \lceil \alpha/n \rceil$  is the maximum number of occurrences of keywords at a single text position. When  $\alpha$  or  $\alpha'$  is large, the bound of [4] may be preferable. The drawback of this algorithm is that, to our knowledge, the method used to implement fixed-length gaps, based on maintaining multiple bit queues using word-level parallelism, is not practical.

Note that the above bounds do not include preprocessing time and the  $\log \sigma$ term in them is due to the simulation of the Aho-Corasick automaton for the strings in the patterns.

In this paper we present two new algorithms, based on dynamic programming and bit-parallelism, for the problem of matching a set of gapped patterns. The first algorithm has  $O(n(\log \sigma + g_{w-\text{span}} \lceil k - \ln(\mathcal{P})/w \rceil) + occ)$ -time complexity, where k-len( $\mathcal{P}$ ) is the total number of keywords in the patterns and  $1 \leq g_{w-span} \leq$ w is the maximum number of distinct gap lengths that span a single word in our encoding. This algorithm is preferable only when  $g_{w-\text{span}} \ll w$ . We then show how to improve the time bound to  $O(n(\log \sigma + \log^2 g_{\text{size}}(\mathcal{P})[\text{k-len}(\mathcal{P})/w]) + occ),$ where  $g_{\text{size}}(\mathcal{P})$  is the size of the variation range of the gap lengths. Note that in the case of unit-length keywords we have  $k-\operatorname{len}(\mathcal{P}) = \operatorname{len}(\mathcal{P})$ . This bound is a moderate improvement over the more general bound for regular expressions by Bille and Thorup [4] for  $\log g_{\text{size}}(\mathcal{P}) = o(\sqrt{\log w})$ . This algorithm can also be extended to support character classes with no overhead. The second algorithm

 $<sup>^{5}</sup>$  Note that the number of occurrences of a keyword that occurs in r patterns and in l positions in the text is equal to  $r \times l$ 

Time	Reference
$\overline{O(n\log\sigma + \alpha)}$	Bille et al. [3]
$O(n(\log \sigma + K) + \alpha')$	Haapasalo et al. [9]
$O(n(\log \sigma + \log w \lceil k \cdot \ln(\mathcal{P})/w \rceil) + occ)$	Bille and Thorup [4]
$O(n(\log \sigma + \log^2 g_{\text{size}}(\mathcal{P})[\text{k-len}(\mathcal{P})/w]) + occ)$	This paper
$O(\lceil n/w \rceil \operatorname{len}(\mathcal{P}) + n + occ)$	This paper

**Table 1.** Comparison of different algorithms for the multiple string matching with gapped patterns problem. k-len( $\mathcal{P}$ ) and len( $\mathcal{P}$ ) are the total number of keywords and symbols in the patterns, respectively.  $g_{\text{size}}(\mathcal{P})$  is the size of the variation range of the gap lengths.  $\alpha \leq n$ k-len( $\mathcal{P}$ ) and  $\alpha' \leq n$ k-len( $\mathcal{P}$ ) are the total number of occurrences in the text of keywords and pattern prefixes, respectively.  $K \leq$ k-len( $\mathcal{P}$ ) is the maximum number of suffixes of a keyword that are also keywords.

is based on a different parallelization of the dynamic programming matrix and has  $O(\lceil n/w \rceil \operatorname{len}(\mathcal{P}) + n + occ)$ -time complexity. The advantage of this bound is that it does not depend on the number of distinct gap lengths. However, it is not strictly on-line, because it processes the text w characters at a time and it also depends on  $\operatorname{len}(\mathcal{P})$  rather than on k-len $(\mathcal{P})$ . Moreover, it cannot support character classes without overhead. The proposed algorithms obtain a bound similar to the one of [4], in the restricted case of fixed-length gaps, while being also practical. For this reason, they provide an effective alternative when  $\alpha$  or  $\alpha'$  is large. They are also fast in practice, as shown by experimental evaluation. A comparison of our algorithms with the existing ones is summarized in Table 1.

The rest of the paper is organized as follows. In Section 2 we recall some preliminary notions and elementary facts. In Section 3 we discuss the motivation for our work. In Section 4 we describe the method based on dynamic programming for matching a set of gapped patterns and then in Section 5 and 6 we present the new algorithms based on it. Finally, in Section 7 we present experimental results to evaluate the performance of our algorithms.

# 2 Basic notions and definitions

Let  $\Sigma$  denote an integer alphabet of size  $\sigma$  and  $\Sigma^*$  the Kleene star of  $\Sigma$ , i.e., the set of all possible sequences over  $\Sigma$ . |S| is the length of string S,  $S[i], i \ge 0$ , denotes its (i + 1)-th character, and  $S[i \dots j]$  denotes its substring between the (i + 1)-st and the (j + 1)-st characters (inclusive). For any two strings S and S', we say that S' is a suffix of S (in symbols,  $S' \sqsupseteq S$ ) if  $S' = S[i \dots |S| - 1]$ , for some  $0 \le i < |S|$ .

A gapped pattern P is of the form

$$S_1 \cdot j_1 \cdot S_2 \cdot \ldots \cdot j_{\ell-1} \cdot S_\ell$$

where  $S_i \in \Sigma^*$ ,  $|S_i| \ge 1$ , is the *i*-th string (keyword) and  $j_i \ge 0$  is the length of the gap between keywords  $S_i$  and  $S_{i+1}$ , for  $i = 1, \ldots, \ell$ . We say that P occurs

in a string T at ending position i if

$$T[i-m+1\ldots i] = S_1 \cdot A_1 \cdot S_2 \cdot \ldots \cdot A_{\ell-1} \cdot S_\ell,$$

where  $A_i \in \Sigma^*$ ,  $|A_i| = j_i$ , for  $1 \le i \le \ell - 1$ , and  $m = \sum_{i=1}^{\ell} |S_i| + \sum_{i=1}^{\ell-1} j_i$ . In this case we write  $P \sqsupseteq_g T_i$ . We denote by  $\operatorname{len}(P) = \sum_{i=1}^{\ell} |S_i|$  and k-len $(P) = \ell$ the number of alphabet symbols and keywords in P, respectively. The gapped pattern  $P_i = S_1 \cdot j_1 \cdot S_2 \cdot \ldots \cdot j_{i-1} \cdot S_i$  is the prefix of P of length  $i \le \ell$ . Given a set of gapped patterns  $\mathcal{P}$ , we denote by  $\operatorname{len}(\mathcal{P}) = \sum_{P \in \mathcal{P}} \operatorname{len}(P)$  and k-len $(\mathcal{P}) = \sum_{P \in \mathcal{P}} k$ -len(P) the total number of symbols and keywords in the patterns, respectively.

The RAM model is assumed, with words of size w in bits. We use some bitwise operations following the standard notation as in the C language: &,  $|, \sim, \ll$  for and, or, not and left shift, respectively. The function to compute the position of the most significant non-zero bit of a word x is  $\lfloor \log_2(x) \rfloor$ .

Given a set S of strings over a finite alphabet  $\Sigma$ , the *trie*  $\mathcal{T}$  associated with S is a rooted directed tree, whose edges are labeled by single characters of  $\Sigma$ , such that

- (i) distinct edges out of the same node are labeled by distinct characters,
- (ii) all paths in  $\mathcal{T}$  from the root are labeled by prefixes of the strings in  $\mathcal{S}$ ,
- (iii) for each string S in S there exists a path in  $\mathcal{T}$  from the root which is labeled by S.

Let Q denote the set of nodes of  $\mathcal{T}$ , root the root of  $\mathcal{T}$ , and label(q) the string which labels the path from root to q, for any  $q \in Q$ . The Aho-Corasick (AC) automaton [1]  $(Q, \Sigma, \delta, root, F)$  for the language  $\bigcup_{S \in S} \Sigma^*S$  is induced directly by the trie  $\mathcal{T}$  for S. The set F of final states include all the states q such that the set  $\{S \in S \mid S \supseteq label(q)\}$  of strings in S which are suffixes of label(q) is nonempty. The transition function  $\delta(q, c)$  of the AC automaton is defined as the unique state q' such that label(q') is the longest suffix of  $label(q) \cdot c$ . Let fail(q)be the unique state p such that label(p) is the longest proper suffix of label(q), for any  $q \in Q \setminus \{root\}$ . Any transition  $\delta(q, c)$  can be recursively computed as

$$\delta(q,c) = \begin{cases} \delta_{\mathcal{T}}(q,c) & \text{if } \delta_{\mathcal{T}}(q,c) \text{ is defined}, \\ \delta(fail(q),c) & \text{if } q \neq root, \\ root & \text{otherwise}, \end{cases}$$

where  $\delta_{\mathcal{T}}$  is the transition function of the trie. Given a string T of length n, let  $q_{-1} = root$  and  $q_i = \delta(q_{i-1}, T[i])$  be the state of the AC automaton after reading the prefix  $T[0 \dots i]$  of T, for  $0 \leq i < n$ . If the transitions of the trie are indexed using a balanced binary search tree, the sequence of states  $q_0, \dots, q_{n-1}$ , i.e., the simulation of the AC automaton on T, can be computed in time  $O(n \log \sigma)$ .

### 3 Motivation

Given a DNA sequence and a motif that describes the binding specificities of a given transcription factor, we study the problem of finding all the binding sites in the sequence that match the motif. The traditional model used to represent transcription factor motifs is the Position Weight Matrix (PWM). This model assumes that there is no correlation between positions in the sites, that is, the contribution of a nucleotide at a given position to the total affinity does not depend on the other nucleotides which appear in other positions. The problem of matching the locations in DNA sequences at which a given transcription factor binds to is well studied under the PWM model [14]. Many more advanced models have been proposed to overcome the independence assumption of the PWM (see [2] for a discussion on the most important ones). One approach, common to some models, consists in extending the PWM model by assigning weights to sets of symbol-position pairs rather than to a single pair only. We focus on the Feature Motif Model (FMM) [17] since, to our knowledge, it is the most general one. In this model the TF binding specificities are described with socalled *features*, i.e., rules that assign a weight to a set of associations between symbols and positions. Given a DNA sequence, a set of features and a motif of length m, the matching problem consists in computing the score of each site (substring) of length m in the sequence, where the score of a site is the sum of the weights of all the features that occur in the site. Formally, a *feature* can be denoted as

$$\{(a_1, i_1), \ldots, (a_q, i_q)\} \rightarrow \omega$$

where  $\omega$  is the affinity contribution of the feature and  $a_j \in \{A, C, G, T\}$  is the nucleotide which must occur at position  $i_j$ , for  $j = 1, \ldots, q$  and  $1 \leq i_j \leq m$ . It is easy to transform these rules into new rules where the left side is a gapped pattern: if  $i_1 < i_2 < \ldots < i_q$ , we can induce the following gapped pattern rule

$$(a_1 \cdot (i_2 - i_1 - 1) \cdot \ldots \cdot (i_q - i_{q-1} - 1) \cdot a_q) \rightarrow (i_q, \omega).$$

Note that we maintain the last position  $i_q$  to recover the original feature. This transformation has the advantage that the resulting pattern is position independent. Moreover, after this transformation, different features may share the same gapped pattern. Hence, the matching problem can be decomposed into two components: the first component identifies the occurrences of the groups of features by searching for the corresponding gapped patterns, while the second component computes the score for each candidate site using the information provided by the first component. For a motif of length m, the second component can be easily implemented by maintaining the score for m site alignments simultaneously with a circular queue of length m. Each time a group of features with an associated set of position/weight pairs  $\{(i_1, \omega_1), \ldots, (i_r, \omega_r)\}$  is found at position j in the sequence, the algorithm adds the weight  $\omega_k$  to the score of the alignment that ends at position  $j + m - i_k$  in the sequence, if  $j \ge i_k$ .

# 4 Dynamic Programming

In this section we present a method based on dynamic programming (DP) to search for a set  $\mathcal{P}$  of gapped patterns in a text T of length n. Then, in the next two sections, we show how to parallelize the computation of the DP matrix columnwise and row-wise using word-level parallelism. Let P be a gapped pattern. We define the matrix D of size k-len $(P) \times n$  where

$$D_{l,i} = \begin{cases} 1 & \text{if } P_l \sqsupseteq_g T_i \,, \\ 0 & \text{otherwise} \,, \end{cases}$$

for  $0 \le l < k$ -len(P) and  $0 \le i < n$ . For example, the matrix corresponding to  $P = c \cdot 2 \cdot at \cdot 1 \cdot t, T = atcgctcatat$  is

	a										
c	0	0	1	0	1	0	1	0	0	0	0
at	0	0	0	0	0	0	0	0	1	0	1
c at t	0	0	0	0	0	0	0	0	0	0	1

From the definition of D it follows that the pattern P occurs in T at position i if and only if  $D_{k-\text{len}(P),i} = 1$ . The matrix D can be computed using the recurrence

$$D_{l,i} = \begin{cases} 1 & \text{if } S_l \supseteq T[0 \dots i-1] \text{ and } (l=1 \text{ or } D_{l-1,i-|S_l|-j_{l-1}}=1), \\ 0 & \text{otherwise.} \end{cases}$$

Let  $D^k$  be the matrix of the k-th pattern in  $\mathcal{P}$ . This method can be generalized to multiple patterns by concatenating the matrices  $D^k$  for all the patterns into a single matrix D of size k-len $(\mathcal{P}) \times n$  and adjusting the definitions accordingly. We now sketch the intuition behind the column-wise and row-wise parallelization.

Consider a column-wise computation of D. If, for each  $P \in \mathcal{P}$ , we replace each gap length  $j_i$  in P with  $\overline{j}_i = j_i + |S_{i+1}|$ , for  $i = 1, \ldots, \text{k-len}(P) - 1$ , and let G be the set of distinct gap lengths in  $\mathcal{P}$ , then we have that each column of Ddepends on |G| previous columns. For example, in the case of  $c \cdot 2 \cdot a \cdot 1 \cdot t$ , we have  $\overline{j}_1 = 4, \overline{j}_2 = 2$  and the l-th column depends on columns l - 2 and l - 4. Instead, in the case of  $c \cdot 2 \cdot a \cdot 1 \cdot at$  we have  $\overline{j}_1 = 3, \overline{j}_2 = 3$  and the l-th column depends on column l-3 only. The idea in the column-wise parallelization is to process w cells of a column in  $O(g_{w-\text{span}})$  time, where  $1 \leq g_{w-\text{span}} \leq w$  is the maximum number of distinct gap lengths that span a segment of w cells in a column. The total time to compute one column (n in total) is thus  $O(g_{w-\text{span}}[\text{k-len}(\mathcal{P})/w])$ . We also describe how to obtain an equivalent set of patterns with  $O(\log g_{\text{size}}(\mathcal{P}))$ distinct gap lengths, where  $g_{\text{size}}(\mathcal{P}) = \max G - \min G + 1$ , at the price of  $O(\log g_{\text{size}}(\mathcal{P}))$ new keywords per gap, thus achieving  $O(\log^2 g_{\text{size}}(\mathcal{P})[\text{k-len}(\mathcal{P})/w])$  time.

Consider now a row-wise computation of D. We have that each row of D depends on the previous row only. To perform this computation efficiently, we split, for each  $P \in \mathcal{P}$ , each keyword  $S_i$  in P in  $|S_i|$  unit-length keywords by inserting a 0 gap length between each two consecutive symbols. For example,  $c \cdot 2 \cdot a t \cdot 1 \cdot t$  becomes  $c \cdot 2 \cdot a \cdot 0 \cdot t \cdot 1 \cdot t$  and the corresponding matrix is

	a	t	с	g	c	t	с	a	t	a	t
c	0	0	1	0	1	0	1	0	0	0	0
a	0	0	0	0	0	0	0	1	0	1	0
t	0	0	0	0	0	0	0	0	1	0	1
t	0	0	0	0	0	0	0	0	0	0	1

In this way the number of rows becomes  $\operatorname{len}(\mathcal{P})$ . Then, the idea in the row-wise parallelization is to process w cells of a row in O(1) time. The total time to compute one row ( $\operatorname{len}(\mathcal{P})$  in total) is thus  $O(\lceil n/w \rceil)$ .

### 5 Column-wise parallelization

Let  $P^k$  be the k-th pattern in  $\mathcal{P}$ . We adopt the superscript notation for  $S_i$ ,  $j_i$  and  $P_l$  with the same meaning. We define the set

$$D_i = \{(k,l) \mid P_l^k \sqsupseteq_g T_i\},\$$

of the prefixes of the patterns that occur at position i in T, for i = 0, ..., n-1,  $1 \leq k \leq |\mathcal{P}|$  and  $1 \leq l \leq k$ -len $(P^k)$ . The set  $D_i$  is a sparse representation of the i-th column of the matrix D defined in the previous section. From the definition of  $D_i$  it follows that the pattern  $P^k$  occurs in T at position i if and only if  $(k, k\text{-len}(P^k)) \in D_i$ . For example, if T = accgtaaacg and  $\mathcal{P} = \{cgt \cdot 2 \cdot ac, c \cdot 1 \cdot gt \cdot 3 \cdot c\}$ , we have  $D_1 = \{(2, 1)\}, D_4 = \{(1, 1), (2, 2)\}$  and  $D_8 = \{(1, 2), (2, 1), (2, 3)\}$ and there is an occurrence of  $P^1$  and  $P^2$  at position 8.

Let  $\mathcal{K} = \{1, \ldots, k\text{-len}(\mathcal{P})\}$  be the set of indices of the keywords in  $\mathcal{P}$  and let  $\overline{T}_i \subseteq \mathcal{K}$  be the set of indices of the matching keywords in T ending at position i. The sequence  $\overline{T}_i$ , for  $0 \leq i < n$ , is basically a new text with character classes over  $\mathcal{K}$ . In the case of the previous example we have  $\mathcal{K} = \{cgt_1, ac_2, c_3, gt_4, c_5\}$  and  $\overline{T}_1 = \{ac_2, c_3, c_5\}$ ,  $\overline{T}_4 = \{cgt_1, gt_4\}$  and  $\overline{T}_8 = \{ac_2, c_3, c_5\}$  (we also show the keyword corresponding to each index for clarity).

We replace each pattern  $S_1 \cdot j_1 \cdot S_2 \cdot \ldots \cdot j_{\ell-1} \cdot S_\ell$  in  $\mathcal{P}$  with the pattern  $\overline{S}_1 \cdot \overline{j}_1 \cdot \overline{S}_2 \cdot \ldots \cdot \overline{j}_{\ell-1} \cdot \overline{S}_\ell$ , with unit-length keywords over the alphabet  $\mathcal{K}$ , where  $\overline{S}_i \in \mathcal{K}$  and  $\overline{j}_i = j_i + |S_{i+1}|$ , for  $1 \leq i < \ell$ . For  $\mathcal{P} = \{cgt \cdot 2 \cdot ac, c \cdot 1 \cdot gt \cdot 3 \cdot c\}$ , the new set is  $\{cgt_1 \cdot 4 \cdot ac_2, c_3 \cdot 3 \cdot gt_4 \cdot 4 \cdot c_5\}$ .

The sets  $D_i$  can be computed using the following lemma:

**Lemma 1.** Let  $\mathcal{P}$  and T be a set of gapped patterns and a text of length n, respectively. Then  $(k,l) \in D_i$ , for  $1 \leq k \leq |\mathcal{P}|$ ,  $1 \leq l \leq k$ -len $(\mathcal{P}^k)$  and  $i = 0, \ldots, n-1$ , if and only if

$$(l = 1 \text{ or } (k, l-1) \in D_{i-\bar{j}_{l-1}^{k}}) \text{ and } S_{l}^{k} \in \bar{T}_{i}.$$

The idea is to match the transformed patterns against the text  $\overline{T}$ . Let  $g_{\min}(\mathcal{P})$ and  $g_{\max}(\mathcal{P})$  denote the minimum and maximum gap length in the patterns, respectively. We also denote with  $g_{\text{size}}(\mathcal{P}) = g_{\max}(\mathcal{P}) - g_{\min}(\mathcal{P}) + 1$  the size of the variation range of the gap lengths. We now present how to efficiently compute any column  $D_i$  using Lemma 1 and word-level parallelism.

Let Q denote the set of states of the AC automaton for the set of distinct keywords in  $\mathcal{P}$ . We store for each state q a pointer  $f_o(q)$  to the state q' such that label(q') is the longest suffix of label(q) that is also a keyword, if any. Let

$$B(q) = \{(k,l) \mid S_l^k \supseteq label(q)\}$$

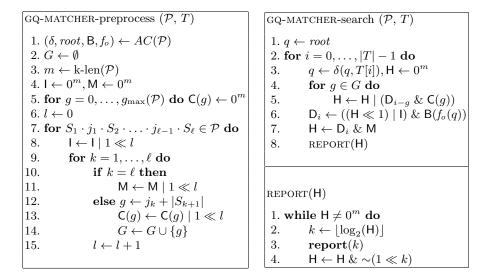


Fig. 1. The GQ-MATCHER algorithm.

be the set of all the occurrences of keywords in the patterns in  $\mathcal{P}$  that are suffixes of label(q), for any  $q \in Q$ . We preprocess B(q) for each state q such that label(q)is a keyword and compute it for any other state using  $B(f_o(q))$ . The sets B can be preprocessed as follows: each time we add to the AC automaton a keyword with index (k, l) and corresponding state q, we first initialize B(q) to  $\emptyset$ , if q is created during the insertion of this keyword, and then add (k, l) to B(q). After the AC automaton is built, we perform a breadth-first traversal of the states of the automaton, and for each state q visited such that label(q) is a keyword we set  $B(q) = B(q) \cup B(f_o(q))$ . It is not hard to see that  $B(f_o(q_i))$  encodes the set  $\overline{T}_i$ , where  $q_i$  is the state of the AC automaton after reading the prefix  $T[0 \dots i]$ of T.

We describe next how to compute any set  $D_i$  using word-level parallelism. Let G be the set of all the distinct gap lengths in the patterns. In addition to the sets B(q), we preprocess also a set C(g), for each  $g \in G$ , defined as follows:

$$C(g) = \{(k,l) \mid j_l^{\kappa} = g\},\$$

for  $1 \leq k \leq |\mathcal{P}|$  and  $1 \leq l < k - len(\mathcal{P}^k)$ . For example, for the set  $\{cgt_1 \cdot 4 \cdot ac_2, c_3 \cdot 3 \cdot gt_4 \cdot 4 \cdot c_3\}$  we have  $C(4) = \{(1, 1), (2, 2)\}$  and  $C(3) = \{(2, 1)\}$ . We encode the sets  $D_i$ , B(q) and C(g) as bit-vectors of k-len( $\mathcal{P}$ ) bits. The generic element (k, l) is mapped onto bit  $\sum_{i=1}^{k-1} k - len(\mathcal{P}^i) + k - len(\mathcal{P}^k_{l-1})$ , where k-len $(\mathcal{P}^k_0) = 0$  for any k. We denote with  $\mathsf{D}_i$ ,  $\mathsf{B}(q)$  and  $\mathsf{C}(g)$  the bit-vectors representing the sets  $D_i$ , B(q) and C(g), respectively. We also compute two additional bit-vectors I and M, such that the bit corresponding to the element (k, 1) in I and  $(k, k - len(\mathcal{P}^k))$  in M is set to 1, for  $1 \leq k \leq |\mathcal{P}|$ . We basically mark the first and the last bit of each pattern, respectively. Let  $\mathsf{H}_i$  be the bit-vector equal to the bitwise or of

the bit-vectors

$$\mathsf{D}_{i-g} \& \mathsf{C}(g), \tag{1}$$

for each  $g \in G$ . Then the corresponding set  $H_i$  is equal to

$$\bigcup_{g\in G} \left\{ (k,l) \mid (k,l) \in D_{i-g} \wedge \overline{j}_l^k = g \right\}.$$

The bit-vector  $D_i$  can then be computed using the following bitwise operations:

$$\mathsf{D}_i \leftarrow ((\mathsf{H}_i \ll 1) \mid \mathsf{I}) \& \mathsf{B}(f_o(q_i))$$

which correspond to the relation

$$\{(k,l) \mid ((k,l-1) \in H_i \lor l = 1) \land (k,l) \in B(f_o(q_i))\}$$

To report all the patterns that match at position i it is enough to iterate over all the bits set in  $D_i$  & M. The algorithm, named GQ-MATCHER, is given in Figure 1.

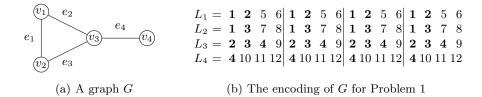
The bit-vector  $\mathsf{H}_i$  can be constructed in time  $O(g_{w\text{-span}}[k\text{-len}(\mathcal{P})/w]), 1 \leq g_{w\text{-span}} \leq w$ , as follows: we compute Equation 1 for each word of the bit-vector separately, starting from the least significant one. For a given word with index j, we have to compute equation 1 only for each  $g \in G$  such that the j-th word of C(g) has at least one bit set. Each position in the bit-vector is spanned by exactly one gap, so the number of such g is at most w. Hence, if we maintain, for each index j, the list  $G_j$  of all the distinct gap lengths that span the positions of the j-th word, we can compute  $\mathsf{H}_i$  in time  $\sum_{j=1}^{\lceil k\text{-len}(\mathcal{P})/w \rceil} |G_j|$ , which yields the advertised bound by replacing  $|G_j|$  with  $g_{w\text{-span}} = \max_j |G_j|$ .

The bit-vectors  $\mathsf{B}(f_o(q_i))$  encoding the sets  $\overline{T}_i$ , for  $0 \leq i < n$ , can be computed in  $O(n \log \sigma)$  time using the AC automaton for the set of distinct keywords in  $\mathcal{P}$ . Given the bit-vectors  $\mathsf{H}_i$  and  $\mathsf{B}(f_o(q_i))$ , the bit-vector  $\mathsf{D}_i$  can be computed in  $O([k-\mathrm{len}(\mathcal{P})/w])$  time. The time complexity of the searching phase of the algorithm is then  $O(n(\log \sigma + g_{w-\mathrm{span}}[k-\mathrm{len}(\mathcal{P})/w]) + occ)$ .

The AC automaton requires  $\Theta(\operatorname{len}(\mathcal{P}))$  space. Moreover, for the recursion of Lemma 1, the algorithm needs to keep the sets D computed in the last  $g_{\max}(\mathcal{P})$  iterations. The lists  $G_j$  require  $O(\operatorname{k-len}(\mathcal{P}) + \lceil \operatorname{k-len}(\mathcal{P})/w \rceil)$  space in total. Finally, the number of B sets (which corresponds to the number of distinct keywords) is  $\leq \operatorname{k-len}(\mathcal{P})$  while the number of C sets is  $\leq g_{\max}(\mathcal{P})$ . Hence, the space complexity is  $O(\operatorname{len}(\mathcal{P}) + (g_{\max}(\mathcal{P}) + \operatorname{k-len}(\mathcal{P}))\lceil \operatorname{k-len}(\mathcal{P})/w \rceil)$ .

Observe that the size of the sets  $G_j$  depends also on the ordering of the patterns (unless k-len(P) is a multiple of w for each  $P \in \mathcal{P}$ ), since more than one pattern can be packed into the same word. Hence, it can be possibly reduced by finding an ordering that maps onto the same word patterns that share many gap lengths. We now show that the problem of minimizing  $\sum_j |G_j|$  is hard. In order to formally define the problem, we introduce the following definition:

**Definition 1.** Let  $L_1, L_2, \ldots, L_n$  be a sequence of lists of integers and let  $L_c$  be the list resulting from their concatenation, say  $L_c = l_1, \ldots, l_{|L_c|}$ . For a given integer b, we define the b-mapping of the lists as the sequence of lists  $L_1^b, L_2^b, \ldots, L_r^b$ 



**Fig. 2.** The reduction of the Hamiltonian Path Problem to Problem 1. The encoding of the graph G with n = 4 vertices and m = 4 edges has  $U = \{1, \ldots, m\} \cup \{m + 1, \ldots, n^2 - m\}$ , and for every vertex  $v_i$ , there is a list  $L_i$  made up of n copies of a sublist of length m consisting of the indices of its incident edges plus some unique symbols from  $\{m+1, \ldots, n^2 - m\}$ ; we take b = (n+1)m and M = (2m-1)(n-1)+m.

where  $r = \lceil |L_c|/b \rceil$ , list  $L_i^b$  contains the elements  $l_{(i-1)b+1}, l_{(i-1)b+2}, \ldots, l_{(i-1)b+b}$ of  $L_c$ , for  $1 \le i \le \lfloor |L_c|/b \rfloor$ , and, if  $r > \lfloor |L_c|/b \rfloor$ , list  $L_r^b$  contains the elements  $l_{(r-1)b+1}, l_{(r-1)b+2}, \ldots, l_{(r-1)b+(|L_c| \mod b)}$ .

Then, the problem of minimizing  $\sum_{j} |G_{j}|$  can be stated as (where in our case we have  $n = |\mathcal{P}|, b = w, U = G$  and  $L_{k} = j_{1}^{k}, j_{2}^{k}, \dots, j_{k-\ln(\mathcal{P}^{k})}^{k}$ , for  $1 \leq k \leq |\mathcal{P}|$ ):

Problem 1 (Permutation with Minimum Distinct Binned Symbols, PMDBS). Given a sequence of n lists of integers  $L_1, L_2, \ldots, L_n$  over a universe U, and an integer b, find the permutation  $\pi$  of  $1, \ldots, n$  which minimizes the sum, over all lists  $L^b$  in the b-mapping of  $L_{\pi(1)}, \ldots, L_{\pi(n)}$ , of the number of distinct elements in  $L^b$ .

We claim that problem PMDBS is intractable (the full proof is in the Appendix):

#### **Theorem 1.** Problem PMDBS is NP-hard in the strong sense.

**Outline of the proof.** We reduce from the Hamiltonian Path Problem (see [7] for basic notions and definitions). In the decision version of the Problem PMDBS, we ask for a permutation  $\pi$  of  $1, \ldots, n$  such that the sum, over all lists  $L^b$  in the *b*-mapping of  $L_{\pi(1)}, \ldots, L_{\pi(n)}$ , of the number of distinct elements in  $L^b$  is at most a given number M.

The idea behind our reduction is that, given a graph G with n vertices, the vertices of G will be encoded by lists, where the list of a vertex consists of the indices of the edges incident to it, under a suitable encoding (see Fig. 2 for an example). This encoding will be such that, choosing M suitably, a permutation of  $1, \ldots, n$  satisfying the bound M corresponds to a Hamiltonian Path in G and vice versa.

We now show how to improve the time complexity in the worst-case by constructing an equivalent set of patterns with  $O(\log g_{\text{size}}(\mathcal{P}))$  distinct gap lengths. Given a set  $S \subset \mathbb{N}$ , a set  $X \subset \mathbb{N}$  is a  $\gamma$ -generating set of S if every element of S can be expressed as the sum of at most  $\gamma$ , non necessarily distinct, elements of X. Suppose that X is a  $\gamma$ -generating set of G. We augment the alphabet  $\Sigma$  with a wildcard symbol \* that matches any symbol of the original alphabet and define the function

$$\phi(g) = (i_1 - 1) \cdot * \cdot (i_2 - 1) \cdot * \cdot \ldots \cdot (i_{l-1} - 1) \cdot * \cdot i_l,$$

for  $g \in G$ , where  $\{i_1, i_2, \ldots, i_l\}$  is an arbitrary combination with repetitions from X of size  $l \leq \gamma$  which generate g, i.e.,  $\sum_{j=1}^{l} i_j = g$ . The function  $\phi$  maps a gap length g onto a concatenation of l gap lengths from the set  $X \cup \{i-1 \mid i \in X\}$  and l-1 wildcard symbols. For example, if  $G = \{1, 2, 5, 6, 10\}$  then  $X = \{1, 5\}$  is a 2-generating set of G and

$$\begin{array}{l} \phi(1) = 1 \\ \phi(2) = \phi(1+1) = 0 \cdot * \cdot 1 \\ \phi(5) = 5 \\ \phi(6) = \phi(1+5) = 0 \cdot * \cdot 5 \\ \phi(10) = \phi(5+5) = 4 \cdot * \cdot 5 \end{array}$$

We generate a new set of patterns  $\mathcal{P}'$  from  $\mathcal{P}$ , by transforming each pattern  $\bar{S}_1 \cdot \bar{j}_1 \cdot \bar{S}_2 \cdot \ldots \cdot \bar{j}_{\ell-1} \cdot \bar{S}_{\ell}$  in  $\mathcal{P}$  into the equivalent pattern

$$\bar{S}_1 \cdot \phi(\bar{j}_1) \cdot \bar{S}_2 \cdot \ldots \cdot \phi(\bar{j}_{\ell-1}) \cdot \bar{S}_\ell$$

In the next subsection we describe how to extend the algorithm presented above to support character classes and therefore also wildcard symbols, since a wildcard is equivalent to a character class containing all the symbols in  $\Sigma$ . By definition of  $\phi$  we have that k-len( $\mathcal{P}'$ )  $< \gamma$ k-len( $\mathcal{P}$ ), since the number of gaps that are split is at most k-len( $\mathcal{P}$ )  $- |\mathcal{P}|$  and the number of wildcard symbols that are added per gap is at most  $\gamma - 1$ . The number of words needed for a bit-vector is then  $< \lceil \gamma \text{k-len}(\mathcal{P})/w \rceil \leq \gamma \lceil \text{k-len}(\mathcal{P})/w \rceil$ . Moreover, the set G' of distinct gap lengths in  $\mathcal{P}'$  is contained in  $X \cup \{i - 1 \mid i \in X\}$  and so its cardinality is O(|X|). This construction thus yields a  $O(n(\log \sigma + |X|\gamma \lceil \text{k-len}(\mathcal{P})/w \rceil) + occ)$  bound, which depends on the generating set used.

W.l.o.g. we assume that  $g_{\max}(\mathcal{P})$  is a power of two (if it is not, we round it up to the nearest power of two). Any positive integer  $g \leq g_{\max}(\mathcal{P})$  can be expressed as a sum of distinct positive powers of two, i.e., the binary encoding of g, such that the largest power of two is  $\leq 2^{\log g_{\max}(\mathcal{P})}$ . This implies that the set  $X = \{0\} \cup \{2^i \mid 0 \leq i \leq \log g_{\max}(\mathcal{P})\}$  is a  $(\log g_{\max}(\mathcal{P}) + 1)$ -generating set of G(we include 0 in X because G may contain 0). For example, if  $G = \{1, 2, 5, 6, 10\}$ then  $X = \{2^i \mid 0 \leq i \leq 3\}$  and

$$\begin{split} \phi(1) &= 1\\ \phi(2) &= 2\\ \phi(5) &= \phi(2^0 + 2^2) = 0 \cdot * \cdot 4\\ \phi(6) &= \phi(2^1 + 2^2) = 1 \cdot * \cdot 4\\ \phi(10) &= \phi(2^1 + 2^3) = 1 \cdot * \cdot 8 \end{split}$$

This generating set yields a  $\log^2 g_{\max}(\mathcal{P})$  factor in the bound, since  $|X| = \log g_{\max}(\mathcal{P}) + 2$  and  $\gamma = \log g_{\max}(\mathcal{P}) + 1$ . We now show how to further improve the bound. Any integer  $g_{\min}(\mathcal{P}) \leq g \leq g_{\max}(\mathcal{P})$  can be written as  $g_{\min}(\mathcal{P}) + g'$ , where  $0 \leq g' \leq g_{\text{size}}(\mathcal{P})$ . Hence, based on the reasoning above, the set  $\{g_{\min}(\mathcal{P})\} \cup \{2^i \mid 0 \leq i \leq \log g_{\text{size}}(\mathcal{P})\}$  is a  $(\log g_{\text{size}}(\mathcal{P}) + 2)$ -generating set of G. We thus obtain the following result:

**Theorem 2.** Given a set  $\mathcal{P}$  of gapped patterns and a text T of length n, all the occurrences in T of the patterns in  $\mathcal{P}$  can be reported in time  $O(n(\log \sigma + \log^2 g_{\text{size}}(\mathcal{P})[\text{k-len}(\mathcal{P})/w]) + occ)$ .

#### 5.1 Character classes

In this subsection we describe how to extend the GQ-MATCHER algorithm to support character classes in the patterns. Let

$$X_1 \cdot j_1 \cdot X_2 \cdot \ldots \cdot j_{\ell-1} \cdot X_\ell$$

be a gapped pattern with character classes, where the keyword  $X_i$  is either a string or a character class, i.e., a subset of  $\Sigma$ . We again replace each pattern  $X_1 \cdot j_1 \cdot X_2 \cdot \ldots \cdot j_{\ell-1} \cdot X_\ell$  with the pattern  $\bar{X}_1 \cdot \bar{j}_1 \cdot \bar{X}_2 \cdot \ldots \cdot \bar{j}_{\ell-1} \cdot \bar{X}_\ell$  with unit-length keywords over the alphabet  $\{1, \ldots, k\text{-len}(\mathcal{P})\}$ , where  $\bar{j}_i = j_i$  if  $X_i$  is a character class. Let  $S_i$  be the set including  $X_i$  itself if  $X_i$  is a string and all the symbols in  $X_i$  otherwise. A keyword  $X_i$  matches in T at ending position i, i.e.,  $\bar{X}_i \in \bar{T}_i$ , if there is a string  $S \in S_i$  such that  $S \supseteq T[0 \ldots i]$ . Observe that Lemma 1 can be used as it is. We build the AC automaton for the set  $\bigcup S_l^k$ , for  $1 \leq k \leq |\mathcal{P}|$  and  $1 \leq l \leq k\text{-len}(\mathcal{P}^k)$ . To support this generalized pattern it is enough to change the definition of the sets B(q) as follows:

$$B(q) = \{(k,l) \mid \exists S \in \mathcal{S}_l^k : S \sqsupseteq label(q)\}.$$

Note that all the strings in a given set  $S_l^k$  are mapped onto the same index (k, l). The algorithm (including the computation of the sets B(q)) does not require any change. Since we add  $\sigma$  distinct strings at most in total for the character classes, the number of B sets is  $\leq k \cdot \operatorname{len}(\mathcal{P}) + \sigma$  and thus we have an  $O(\sigma \lceil k \cdot \operatorname{len}(\mathcal{P})/w \rceil)$ overhead in the preprocessing time and space complexity.

#### 6 Row-wise parallelization

We now describe the row-wise parallelization of the DP matrix, based on the ideas of the  $(\delta, \alpha)$ -matching algorithm described in [5]. This algorithm works for a single pattern only, thus to solve the multi-pattern case we need to run (the search phase of) the algorithm several times. In this algorithm we take a different approach to handle arbitrary length keywords. In particular, we first

GQ-MATCHER-T $(\mathcal{P}, T)$
. for $s \in \Sigma$ do $V[s] \leftarrow 0$
2. for $c \leftarrow 0$ to $\lceil n/w \rceil$ do
B. for $i \leftarrow cw$ to $\min(n, (c+1)w) - 1$ do $V[T[i]] \leftarrow V[T[i]] \mid (1 \ll (i \mod w))$
$\mathbf{for} \ k \leftarrow 1 \ \mathbf{to} \  \mathcal{P}  \ \mathbf{do}$
5. $D_{1,c}^{k,w} \leftarrow V[p_1^k]$
5. for $r \leftarrow 2$ to $\operatorname{len}(P^k)$ do $D_{r,c}^{k,w} \leftarrow V[p_r^k] \& M(k, r-1, c, j_{r-1}+1)$
7. REPORT $(D_{\mathrm{len}(P^k),c}^{k,w})$
B. for $i \leftarrow cw$ to $\min(n, (c+1)w) - 1$ do $V[T[i]] \leftarrow 0$

Fig. 3. The GQ-MATCHER-T algorithm.

transform each pattern  $S_1 \cdot j_1 \cdot S_2 \cdot \ldots \cdot j_{\ell-1} \cdot S_\ell$  in  $\mathcal{P}$  into the equivalent pattern  $\psi(S_1) \cdot j_1 \cdot \psi(S_2) \cdot \ldots \cdot j_{\ell-1} \cdot \psi(S_\ell)$ , where

$$\psi(S) = \begin{cases} S[0] \cdot 0 \cdot \psi(S[1 \dots |S| - 1]) & \text{if } |S| > 1, \\ S[0] & \text{otherwise,} \end{cases}$$

so that all the keywords have unit length and the number of keywords is  $\operatorname{len}(\mathcal{P})$ . We denote by  $p_r^k$  the *r*-th keyword (symbol) of the *k*-th pattern. We also parallelize over the text, rather than over the set of patterns. The main benefit is that now there is only one gap length to consider at each step. This also means that instead of preprocessing the set of patterns, we now must preprocess the text. For the same reason the algorithm is not strictly on-line anymore, as it processes the text *w* characters at a time.

Let  $D^k$  be the matrix as defined in Section 4 for the k-th pattern in  $\mathcal{P}$  and let  $D^k_{r,c}$  be the cell of  $D^k$  at row r and column c. Observe that in the case of unit-length keywords the recurrence to compute  $D^k$  simplifies to

$$D_{r,c}^{k} = \begin{cases} 1 & \text{if } p_{r}^{k} = T[c] \text{ and } (r = 1 \text{ or } D_{r-1,c-j_{r-1}-1}^{k} = 1), \\ 0 & \text{otherwise.} \end{cases}$$

The matrix  $D^k$  has  $\operatorname{len}(P^k)$  rows and n columns and is easy to compute in  $O(n \operatorname{len}(P^k))$  time using dynamic programming. We now show how it can be computed in  $O(\lceil n/w \rceil \operatorname{len}(P^k))$  time using word-level parallelism by processing chunks of w columns in O(1) time.

To this end, let V be a matrix of size  $\sigma \times n$ , where

$$V_{s,c} = \begin{cases} 1 & \text{if } s = T[c], \\ 0 & \text{otherwise}, \end{cases}$$

for  $s \in \Sigma$  and  $0 \leq c < n$ . Let also  $\Sigma_{\mathcal{P}}$  be the subset of  $\Sigma$  of size  $\sigma_{\mathcal{P}} \leq \min(\sigma, \operatorname{len}(\mathcal{P}))$  of the symbols occurring in the patterns. Assume that we have the rows of V which correspond to the symbols of  $\Sigma_{\mathcal{P}}$  encoded in an array of  $\sigma$ 

bit-vectors of  $\lceil n/w \rceil$  bits. The entries corresponding to symbols not in  $\Sigma_{\mathcal{P}}$  are not initialized. The set  $\Sigma_{\mathcal{P}}$  can be trivially computed in  $O(\operatorname{len}(\mathcal{P})\log \sigma_{\mathcal{P}})$  time using a binary search tree. The array can be computed in  $O(\lceil n/w \rceil \sigma_{\mathcal{P}} + n)$  time.

The computation of  $D^k$  will proceed row-wise, w columns at once, as each matrix element takes only one bit of storage and we can store w columns into a single machine word. We adopt the notation  $\mathsf{D}_{r,c}^{k,w} = D_{r,cw...(c+1)w-1}^k$ , and analogously for V. First notice that by definition  $\mathsf{D}_{1,c}^{k,w} = \mathsf{V}_{p_1^k,c}^w$ . Assume now that the words  $\mathsf{D}_{r-1,c'}^{k,w}$  for  $c' \leq c$  have been already computed, and we want to compute  $\mathsf{D}_{r,c}^{k,w}$ . To do so, we need to check if any text character in the current chunk  $T[cw\ldots(c+1)w-1]$  matches the pattern character  $p_r^k$  (readily solved as  $\mathsf{V}_{p_r^k,c}^w$ ), and if  $g = j_{r-1} + 1$  text characters back there was a matching pattern prefix of length r-1. The corresponding bits signaling these prefix matches, relevant to the current chunk, are distributed in at most two consecutive words in a w-bit wide interval in the previous row, namely in words  $\mathsf{D}_{r-1,c'-1}^{k,w}$  and  $\mathsf{D}_{r-1,c'}^{k,w}$ , where  $c' = c - \lfloor g/w \rfloor$ . We select the relevant bits and combine them into a single word using the following function:

$$M(k,r,c,g) = (\mathsf{D}^{k,w}_{r,c-\lfloor g/w \rfloor - 1} \gg (w - (g \bmod w))) \mid (\mathsf{D}^{k,w}_{r,c-\lfloor g/w \rfloor} \ll (g \bmod w)).$$

The recurrence can now be written as

$$\mathsf{D}_{r,c}^{k,w} \leftarrow \mathsf{V}_{p_r^k,c}^w \& M(k,r-1,c,j_{r-1}+1),$$

and  $D^k$  can be computed in  $O(\lceil n/w \rceil \operatorname{len}(P^k))$  time for any k. To check the occurrences, we just scan the last row of the matrix and report every position where the bit is 1. To handle all the patterns, we run the search algorithm  $|\mathcal{P}|$  times, which gives  $O(\lceil n/w \rceil \operatorname{len}(\mathcal{P}) + n + occ)$  total time, including the preprocessing. The algorithm needs  $O(\sigma + \lceil g_{\max}(\mathcal{P})/w \rceil \max_k(\operatorname{len}(P^k)))$  words of space, as only the current column of  $\mathsf{V}^w$  and the last  $O(\lceil g_{\max}(\mathcal{P})/w \rceil)$  columns of  $\mathsf{D}^{k,w}$  need to be kept in memory at any given time.

Based on the observation that we need only the rows of V corresponding to the symbols in  $\Sigma_{\mathcal{P}}$ , we can also manage to reduce the space for V from  $O(\sigma)$ to  $O(\min(\sigma_{\mathcal{P}}, w) + \lceil \sigma/w \rceil)$  words. First, we build a (constant time) mapping  $\mu$ from  $\Sigma_{\mathcal{P}}$  to  $\{1, \ldots, \sigma_{\mathcal{P}}\}$ . One (practical) way to compute  $\mu$  is to encode  $\Sigma_{\mathcal{P}}$  in a bit-vector **S** of  $\sigma$  bits and build a rank dictionary [11] for it. The rank dictionary allows one to compute the function  $rank_1(\mathbf{S}, i)$  which returns the number of bits set to 1 among the first i positions in **S**. In this way the mapping can be implemented as  $\mu(s) = rank_1(\mathbf{S}, s)$ . The rank dictionary can be built in  $O(\sigma)$ time and requires  $O(\lceil \sigma/w \rceil)$  space. We can then encode V using  $O(\sigma_{\mathcal{P}})$  words and access the row corresponding to any symbol  $s \in \Sigma_{\mathcal{P}}$  as  $V[\mu(s)]$ . If  $w < \sigma_{\mathcal{P}}$ we can further reduce the space for V by exploiting the fact that we process Tin chunks. The idea is to compute, for a given chunk of T of length w starting at position c, a bit-vector  $\mathbf{S}'$  of  $\sigma_{\mathcal{P}}$  bits where we set bit  $\mu(s)$  for each  $s \in \Sigma_{\mathcal{P}}$  which occurs in the chunk. Note that if s does not occur in the chunk then  $V_{s,c}^w = 0$ . By building a rank dictionary for  $\mathbf{S}'$  we obtain a mapping from the subset of  $\Sigma_{\mathcal{P}}$  encoded in S' to  $\{1, \ldots, w\}$ , i.e.,  $rank_1(\mathbf{S}', \mu(s))$  is the mapping for symbol s. We can then encode V using O(w) words and access the row corresponding to any symbol  $s \in \Sigma_{\mathcal{P}}$  as  $V[rank_1(\mathbf{S}', \mu(s))]$ , if bit  $\mu(s)$  is set in S', and as a word equal to 0 otherwise. Observe that there are  $\lceil n/w \rceil$  chunks; the time to compute any bit-vector S' and its rank dictionary is  $O(w + \sigma_{\mathcal{P}})$ . Hence, we spend  $O(\lceil n/w \rceil \sigma_{\mathcal{P}} + n)$  time in total and maintain the original time complexity. Alternatively, we can reduce the space for V to  $O(\sigma_{\mathcal{P}})$  by computing  $\mu$  using Ružić's dictionary [16] for  $\Sigma_{\mathcal{P}}$ , whose construction requires  $O(\sigma_{\mathcal{P}}(\log \log \sigma_{\mathcal{P}})^2)$  time.

The algorithm, named GQ-MATCHER-T, is given in Figure 3. We thus obtain the following result:

**Theorem 3.** Given a set  $\mathcal{P}$  of gapped patterns and a text T of length n, given in chunks of w characters, all the occurrences in T of the patterns in  $\mathcal{P}$  can be reported in time  $O(\lceil n/w \rceil \operatorname{len}(\mathcal{P}) + n + \operatorname{occ})$ .

## 7 Experimental results

The proposed algorithms have been experimentally validated. In particular, we compared the new algorithms GQ-MATCHER, GQ-MATCHER-T with the D-PMA algorithm of [9] and the L-PMA algorithm of [3]. The GQ-MATCHER and GQ-MATCHER-T have been implemented in the C++ programming language and compiled with the GNU C++ Compiler 4.6, using the options -O3. The source code of the D-PMA algorithm was kindly provided by the authors. The test machine was a 3.00 GHz Intel Core 2 Quad Q9650 running Ubuntu 12.04 and running times were measured with the getrusage function. The benchmarks consisted of searching for a set of randomly generated gapped patterns in the DNA sequence of 4,638,690 base pairs of the Escherichia coli genome  $(\sigma = 4)^6$  and in the protein sequence of 2,922,023 symbols of the Saccharomyces cerevisiae genome  $(\sigma = 20)^7$ . The patterns were generated using the following procedure: given the number k of keywords, the length l of each keyword and the maximum length b of a gap, we first randomly generate a sequence  $g_1, g_2, \ldots, g_{l-1}$  of l-1gap lengths in the interval [0, b]; then, we randomly sample a string of length  $k \times l + \sum_{i=1}^{l-1} g_i$  from the text, and replace the substrings corresponding to the gaps with their lengths. Figures 4 and 5 show the experimental results for the DNA and protein sequence, respectively. For each sequence, we performed the following experiments:

- 1. (top row of Figures 4 and 5) searching a set of gapped patterns with 6 keywords of unit length with a fixed number of patterns equal to 50 and 100, respectively, and such that the maximum gap varies between 5 and 60;
- 2. (middle row of Figures 4 and 5) searching a set of gapped patterns with 6 keywords of unit length with a fixed maximum gap of 20 and 40, respectively, and such that the number of patterns varies between 25 and 200;

<sup>&</sup>lt;sup>6</sup> http://corpus.canterbury.ac.nz/

<sup>&</sup>lt;sup>7</sup> http://www.yeastgenome.org/

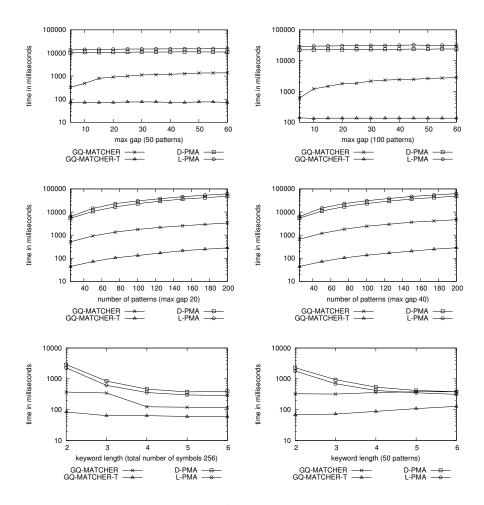


Fig. 4. Experimental results on the DNA sequence of the *Escherichia coli* genome with randomly generated gapped patterns. Top row: 6 unit-length keywords, varying gap interval with a set of 50 and 100 patterns; Middle row: 6 unit-length keywords, varying number of patterns with maximum gap 20 and 40; Bottom row: 2 keywords, varying keyword length.

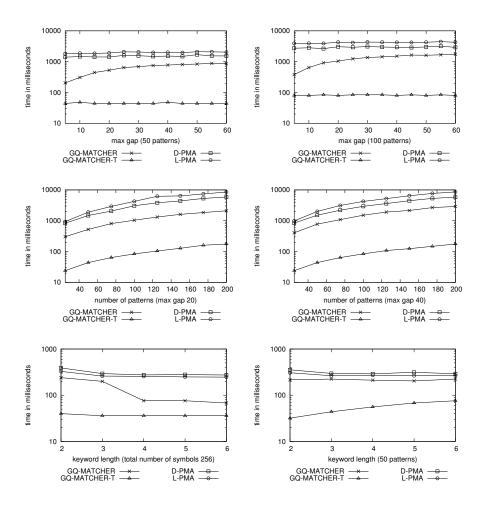


Fig. 5. Experimental results on the protein sequence of the *Saccharomyces cerevisiae* genome with randomly generated gapped patterns. Top row: 6 unit-length keywords, varying gap interval with a set of 50 and 100 patterns; Middle row: 6 unit-length keywords, varying number of patterns with maximum gap 20 and 40; Bottom row: 2 keywords, varying keyword length.

3. (bottom row of Figures 4 and 5) searching a set of gapped patterns with 2 keywords and a fixed maximum gap of 20 and such that the keyword length varies between 2 and 6. In the benchmark to the left the number of patterns is calculated using the formula 4w/2l, where l is the keyword length, so as to fix the total number of symbols, i.e.,  $len(\mathcal{P})$ , to 4w (i.e., 4 words in our algorithm). In the one to the right the number of patterns is fixed to 50, so that  $len(\mathcal{P})$  increases as the keyword length grows.

We used a logarithmic scale on the y axis. Note that the number of words used by our algorithm is equal to  $\lceil 6 \times |\mathcal{P}|/w \rceil$ , so it is between 3 and 19 in our experiments since w = 64. Concerning the benchmark on DNA, the experimental results show that the new algorithms are significantly faster (up to 50 times) than the D-PMA and L-PMA algorithms in the case of unit-length keywords (top and middle row). in the case of arbitrary length keywords (bottom row), our algorithms are significantly faster than D-PMA and L-PMA up to keyword length 4, while for longer keywords they have similar performance. In the benchmark on the protein sequence the D-PMA and L-PMA algorithms are considerably faster compared to the case of DNA, which is expected since the average value of  $\alpha$  and  $\alpha'$  is inversely proportional to the alphabet size. Instead, our algorithms exhibit a similar behaviour and are still faster than both D-PMA and L-PMA.

The GQ-MATCHER-T algorithm is preferable if the text can be processed by reading w symbols at a time. This implies that, in the worst-case, we report an occurrence of a pattern at position i in the text only after reading the symbols up to position i+w-1. This condition may not be feasible for some applications. Otherwise, albeit slower, the GQ-MATCHER algorithm is a good choice.

### 8 Conclusions

Motivated by a problem in computational biology, we have presented new algorithms for the problem of *multiple string matching* of gapped patterns, where a gapped pattern is a sequence of strings such that there is a gap of fixed length between each two consecutive strings. The presented algorithms are based on dynamic programming and bit-parallelism, and lie in a middle-ground among the existing algorithms. In fact, their time complexity is close to the best existing bound and, yet, they are also practical. We have also assessed their performance with experiments and showed that they are fast in practice and preferable if the strings in the patterns have unit-length.

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# A Proof of Theorem 1

**Theorem 1.** Problem PMDBS is NP-hard in the strong sense.

*Proof.* Given an input  $G = (V = \{v_1, \ldots, v_n\}, E = \{e_1, \ldots, e_m\})$  to the Hamiltonian Path Problem, we construct the following instance  $\mathcal{L}_G$  to Problem 1 (see Fig. 2 for an example).

- The universe U consists of numbers  $\{1, \ldots, m\}$ , which will be used to encode adjacencies, and numbers  $\{m+1, \ldots, n^2-m\}$ , which will be used for padding, to ensure that all lists have the same length.
- For every vertex  $v_i \in V$ , we have a list  $L_i$  constructed as follows. Suppose the incident edges of  $v_i$  are  $e_{i_1}, e_{i_2}, \ldots, e_{i_t}$ , and say that the basic list of  $L_i$  is the list  $i_1, i_2, \ldots, i_t$  padded (at the end) with m - t new numbers from  $\{m + 1, \ldots, n^2 - m\}$ , unused by any other list. List  $L_i$  consists of nconcatenated copies of its basic list, so that  $|L_i| = nm$ .
- We set b = (n+1)m and M = (2m-1)(n-1) + m.

We show that G has a Hamiltonian path if and only if instance  $\mathcal{L}_G$  admits a permutation  $\pi$  of  $1, \ldots, n$  such that the sum, over all lists  $L^b$  in the b-mapping of  $L_{\pi(1)}, \ldots, L_{\pi(n)}$ , of the number of distinct elements in  $L^b$  is at most M. Since the values of the integers in U are bounded by a polynomial in the size of the lists  $L_1, \ldots, L_n$ , this claim will entail the NP-hardness in the strong sense of Problem PMDBS.

First, observe that from the choice of b and of the lengths of lists  $L_i$ , for any permutation  $\pi$  of  $1, \ldots, n$ , the b-mapping  $L_1^b, \ldots, L_r^b$  of  $L_{\pi(1)}, L_{\pi(2)}, \ldots, L_{\pi(n)}$ has a special form. Indeed, since b = (n+1)m, and the length of the lists  $L_i$ is nm, we have that  $r = \lceil (n^2m)/((n+1)m) \rceil = \lceil n^2/(n+1) \rceil = n$ . It can be easily shown by induction that, for all  $1 \le j \le n-1$ , list  $L_j^b$  consists of the last (n-j+1)m integers in the list  $L_{\pi(j)}$  followed by the first jm integers from the list  $L_{\pi(j+1)}$ . List  $L_n^b$  consists of the last m integers of list  $L_{\pi(n)}$ .

For the forward direction, let  $P = v_{i_1}, \ldots, v_{i_n}$  be a Hamiltonian path of G. We show that the permutation  $\pi$  of  $1, \ldots, n$  defined such that  $\pi(j) = i_j$  satisfies the bound M. Let  $L_1^b, L_2^b, \ldots, L_n^b$  be the b-mapping of  $L_{\pi(1)}, L_{\pi(2)}, \ldots, L_{\pi(n)}$ . From the above observation, for all  $1 \leq j \leq n-1$ , the number of distinct integers in  $L_j^b$  equals the number of distinct integers in  $L_{\pi(j)}$ , which is m, plus the number of distinct integers in  $L_{\pi(j+1)}$ , which is m, minus the number of integers shared between  $L_{\pi(j)}$  and  $L_{\pi(j+1)}$ . Since  $v_{\pi(j)}$  and  $v_{\pi(j+1)}$  are connected by an edge, then the index of this edge appears in both  $L_{\pi(j)}$  and  $L_{\pi(j+1)}$ , thus the number of distinct elements in  $L_j^b$  is at most 2m - 1. The claim is now clear, since  $L_n^b$ consists of m distinct integers.

For the backward implication, let  $\pi$  be a permutation of  $1, \ldots, n$  such that the sum, over all lists  $L^b$  in the *b*-mapping of  $L_{\pi(1)}, \ldots, L_{\pi(n)}$ , of the number of distinct elements in  $L^b$  is at most M. We claim that the sequence  $P = v_{\pi(1)}, \ldots, v_{\pi(n)}$  is a Hamiltonian path in G. Since  $\pi$  is a permutation of  $1, \ldots, n$ , we only have to show that for all  $1 \leq i \leq n-1$ , there is an edge between  $v_{\pi(i)}$  and  $v_{\pi(i+1)}$ . Let  $L_1^b, L_2^b, \ldots, L_n^b$  be the *b*-mapping of  $L_{\pi(1)}, L_{\pi(2)}, \ldots, L_{\pi(n)}$ . The fact that the number of distinct elements in the list  $L_n^b$  is *m* entails that the sum, over all  $1 \leq j \leq n-1$ , of the number of distinct elements in  $L_j^b$  is at most M-m = (2m-1)(n-1). For all  $1 \leq j \leq n-1$ , vertices  $v_{\pi(j)}$  and  $v_{\pi(j+1)}$ have at most one edge incident to both of them (the edge connecting them), therefore, the number of distinct integers in each list  $L_j^b$  is at least 2m-1. From the above observation, for all  $1 \leq j \leq n-1$ , the number of distinct integers in each list  $L_j^b$  is exactly 2m-1.

Since the number of distinct integers in the list  $L_{\pi(j)}$  is m and the number of distinct integers in the list  $L_{\pi(j+1)}$  is m, but the number of distinct integers in  $L_j^b$  is at most 2m - 1, we have that lists  $L_{\pi(j)}$  and  $L_{\pi(j+1)}$  share at least one integer. We padded the basic lists of  $L_{\pi(j)}$  and  $L_{\pi(j+1)}$  with integers unique to them, thus the only integer shared by them must be the index of the edge incident to both  $v_{\pi(j)}$  and  $v_{\pi(j+1)}$ . Such an edge connects  $v_{\pi(j)}$  and  $v_{\pi(j+1)}$ , and thus P is a path in G.