Finding Approximate Palindromes in Strings

Alexandre H. L. Porto Valmir C. Barbosa

Programa de Engenharia de Sistemas e Computação, COPPE
Universidade Federal do Rio de Janeiro
Caixa Postal 68511
21945-970 Rio de Janeiro - RJ, Brazil

xandao@cos.ufrj.br, valmir@cos.ufrj.br

Abstract

We introduce a novel definition of approximate palindromes in strings, and provide an algorithm to find all maximal approximate palindromes in a string with up to k errors. Our definition is based on the usual edit operations of approximate pattern matching, and the algorithm we give, for a string of size n on a fixed alphabet, runs in $O(k^2n)$ time. We also discuss two implementation-related improvements to the algorithm, and demonstrate their efficacy in practice by means of both experiments and an average-case analysis.

Keywords: Approximate palindromes, string editing, approximate pattern matching.

1. Introduction

Let S be a string of n characters from a fixed alphabet Σ . For $1 \leq i \leq j \leq n$, let S[i] denote the ith character in S and S[i..j] denote the substring of S whose first and last characters are S[i] and S[j], respectively. We let S^R denote the string whose ith character is S[n-i+1], that is, S and S^R are essentially the same string when read in opposing directions. We say that S and S^R are the reverse of each other.

In this paper, we are concerned with palindromes occurring in S, which are substrings S[i ... j] such that $S[i ... j] = S[i ... j]^R$. If S[i ... j] is a palindrome, then it is an even palindrome if it contains an even number of characters, otherwise it is an odd palindrome. The center of this palindrome is S[c], where $c = i - 1 + \lceil (j - i + 1)/2 \rceil$. It follows that $S[c + 1 ... j] = S[i ... c]^R$ for an even palindrome, while $S[c + 1 ... j] = S[i ... c - 1]^R$ for an odd palindrome. A palindrome S[i ... j] is an initial palindrome if i = 1 and a final palindrome if j = n. It is said to be a maximal palindrome if it is an initial palindrome, a final palindrome, or if S[i - 1 ... j + 1] is not a palindrome for $1 < i \le j < n$.

Several algorithms have appeared for the detection of palindromes in strings. These include sequential algorithms for detecting all initial palindromes or maximal palindromes centered at all positions [1, 2], as well as parallel algorithms [3–6].

Palindromes appear in several domains, chiefly in computational molecular biology [7, 8], where Σ is for example the set of bases that link together to form strands of nucleic acid. In this domain of application, palindromes are often required to be *complementary*, in the following sense. While for a palindrome centered at c we have either S[c-r+1] = S[c+r] or S[c-r] = S[c+r], depending respectively on whether the palindrome is even or odd and for r representing distance from the center, if the palindrome is complementary then the two characters are no longer equal but rather constitute a complementary pair. In this case, we no longer have $S[i..j] = S[i..j]^R$, but rather complementarity between the two strings.

Although we in the sequel deal exclusively with palindromes for which equality is used to compare them with their reverses (everything carries over trivially to the case of complementarity), we dwell a little longer on the application of palindromes to computational molecular biology because in that area the definition we have given for palindromes is "too exact," being therefore of little use. Palindromes that matter in that domain are "approximate," in the sense that the symmetry around a palindrome's center need not be perfect, but may instead contain a certain number of mismatches in the form of gaps and defects of various other natures [7, 8]. This paper is about finding approximate palindromes in S.

The following is how the balance of this paper is organized. We start in Section 2 by providing a precise definition of what is to be understood as an approximate palindrome and a maximal approximate palindrome. This definition is novel, as previous definitions appear to have been too restricted [7]. Then in Section 3 we give an algorithm to find all maximal approximate palindromes in a string allowing for k errors. The algorithm runs in $O(k^2n)$ time. Section 4 contains two improvements on the basic algorithm. These improvements do not lead to an improved complexity,

but do in practice make a difference, as we demonstrate by means of some experimental results. Section 5 contains an average-case analysis of the two improvements, which indicates that the conclusions drawn in the previous section can be expected to hold on average. Concluding remarks follow in Section 6.

2. Approximate palindromes

Our definition of an approximate palindrome centered at position c in string S is given for an integer $k \geq 0$ indicating the maximum number of errors to be tolerated, and is based on the notion of *string editing*, that is, the transformation of one string into another [7]. In order to define approximate palindromes, we consider, for $1 \leq c \leq n$, the editing of string $S_{\ell}^{c} = S[1 ... u]^{R}$ to obtain string $S_{r}^{c} = S[c+1...n]$, where u = c for even palindromes or u = c-1 for odd palindromes (here, and henceforth, S[i...j] is to be understood as the empty string if i > j).

The string editing that we consider is the same that has been used for other problems on strings, and employs the operations presented next. These operations act on cursors p and q, which are used to point to specific positions in S_{ℓ}^c and S_r^c , respectively. Such cursors are such that $0 \le p \le u$ and $0 \le q \le n - c$, the value 0 being used only to initialize the cursors as still not pointing to characters in the string. Note that p and q, when nonzero, do not indicate positions in S, but in two of its substrings taken as independent entities.

The operations we consider are the following, of which (ii)–(iv) are called *edit operations*.

- (i) Matching: If $S_{\ell}^{c}[p+1] = S_{r}^{c}[q+1]$, then increment both p and q.
- (ii) Substitution: If $S_{\ell}^{c}[p+1] \neq S_{r}^{c}[q+1]$, then increment both p and q.
- (iii) Insertion: Increment q.
- (iv) Deletion: Increment p.

While a matching can only be applied if it will make both cursors point to equal characters, the edit operations characterize the possible sources of mismatch between the two strings. What they do is to allow for a character from S_r^c to substitute for a character in S_ℓ^c (this is a substitution), for a character from S_r^c to be inserted into S_ℓ^c as an additional character (an insertion), or for a character to be deleted from S_ℓ^c (a deletion). When grouped into a sequence, what matching and edit operations can be regarded as doing is providing a script (the *edit script*) for a prefix of S_ℓ^c to be turned into a replica of a prefix of S_r^c (note that, if an unlimited number of edit operations is allowed, then such an edit script is guaranteed to exist). The edit script to convert one prefix into the other having the smallest number of edit operations is said to be *optimal* for the two prefixes, and its number of edit operations is called the *edit distance* between them [9, 10].

For $0 \le p^* \le u$ and $0 \le q^* \le n - c$, we say that $S[u - p^* + 1 \dots c + q^*]$ is an approximate palindrome in S centered at c if, of all the edit scripts that can be used to turn $S_{\ell}^{c}[1 \dots p^*]$ into $S_{r}^{c}[1 \dots q^*]$, the one that is optimal comprises no more than k edit operations (in other words, the edit distance between $S_{\ell}^{c}[1 \dots p^*]$ and $S_{r}^{c}[1 \dots q^*]$ is at most k). In this case, p^* and q^* are the values

of p and q, respectively, after any of those edit scripts is played out. The palindrome is even or odd according to how S_{ℓ}^{c} is originally set. Its *size* is either $p^* + q^*$ or $p^* + q^* + 1$, respectively if it is even or odd. This definition is more general than the single other definition that appears to have been given for approximate palindromes [7], which only allows for matchings and substitutions.

It is curious to observe that, unlike exact palindromes, the size of an even approximate palindrome does not have to be even, nor does the size of an odd approximate palindrome have to be odd. These would hold, however, for the exact palindrome that would be obtained if the transformation of one prefix into the other were indeed performed.

We provide in Figure 1 an illustration of this concept of an approximate palindrome. The figure contains four approximate palindromes in the string bbaabac for k=3, two even in part (a) and two odd in part (b). The palindromes are depicted in a way that evidences their two parts and also their centers, in the odd case. Blank cells appearing in the left part correspond to insertions, those on the right to deletions (for ease of representation, in the figure we let deletions from the left part be represented as insertions into the right part). Substitutions are indicated by shaded cells placed symmetrically in the two parts.

Having defined approximate palindromes for c and k fixed, the notion that remains to be introduced before we move on to discuss their detection is that of maximality. Note, first, that the simple definition of a maximal palindrome in the exact case does not carry over simply to the approximate case. In the case of exact palindromes, maximality is related to the inability to extend a palindrome into another substring of S that is also a palindrome. In the approximate case, however, the potential existence of several acceptable edit scripts makes it inappropriate to adopt such a straightforward definition.

While there does appear to exist more than one possibility for defining the maximality of approximate palindromes, what we do in this paper is to say that an approximate palindrome is maximal if no other approximate palindrome for the same c and k exists having strictly greater size or the same size but strictly fewer errors (edit distance between its two parts). Unlike the case of exact palindromes, this definition clearly does not guarantee the uniqueness of an approximate palindrome that is maximal.

3. An algorithm

In this section, and for k fixed, we introduce an algorithm for detecting maximal approximate palindromes, one even and one odd for each c such that $1 \le c \le n$.

Our algorithm is based on an acyclic directed graph D, whose definition relies on two generic strings X and Y on the same alphabet. We let x = |X| and y = |Y|. Graph D has (x+1)(y+1) nodes, one for each (i,j) pair such that $0 \le i \le x$ and $0 \le j \le y$. A directed edge exists in D from node (i,j) to node (i',j') if either i'=i and j'=j+1, or i'=i+1 and j'=j, or yet i'=i+1 and j'=j+1. If we position the nodes of D on the vertices of a two-dimensional grid having x+1 rows and y+1 columns so that a node's first coordinate grows from top to bottom and the second from left to right, then clearly directed edges exist between nearest neighbors in

the same row (a horizontal edge), the same column (a vertical edge), and the same diagonal (a diagonal edge). Because j' - i' = j - i when a diagonal edge exists from (i, j) to (i', j'), we use such differences to label the various diagonals on the grid. Diagonal labels are then in the range of -x through y.

Now consider a directed path in D leading from node (i,j) to node (i',j'). By definition of the directed edges, clearly $i' \geq i$ and $j' \geq j$. The importance of graph D in our present context is that this directed path, if it contains at least one edge, can be interpreted as an edit script for string X[i+1..i'] to be transformed into string Y[j+1..j']. Along the script, the cursors p and q of operations (i)–(iv) are used on X and Y, respectively, such that $i \leq p \leq i'$ and $j \leq q \leq j'$. On such a path, a diagonal edge corresponds to either a matching or a substitution, a horizontal edge to an insertion, and a vertical edge to a deletion. The number of edges on the path that do not correspond to matchings is the number of edit operations in the script. The optimal edit script for strings X[i+1..i'] and Y[j+1..j'] is represented in D by a directed path from (i,j) to (i',j') whose number of edges corresponding to edit operations is minimum among all directed paths between the two nodes. Such a path is said to be shortest among all those paths according to the metric that assigns, say, length 0 to edges corresponding to matchings and length 1 to all other edges.

We give an illustration in Figure 2, where graph D is shown for X = bb and Y = aabac. The directed path shown in solid lines contains two insertions, followed by one matching and one substitution, and is a shortest path between its two end vertices. It corresponds, therefore, to an optimal edit script to transform X[1..2] into Y[1..4]. All other edges are shown as dotted lines, directions omitted for clarity.

For $0 \le e \le k$, let a directed path in D be called an e-path if it contains e edges related to edit operations. One crucial problem to be solved on D is the problem of determining, for each diagonal and each e, the e-path, if one exists, that starts in row 0, ends on that diagonal at the farthest possible node (greatest row number), and is in addition shortest among all paths that start and end at the same nodes. This problem can be solved by the following dynamic-programming approach.

- 1. For d = 0, ..., y, find the largest common prefix of strings X and Y[d + 1...y]. Such prefixes will correspond to the 0-paths that start in row 0 and end at the farthest possible nodes. Each of them will be entirely confined to a diagonal d and, like all 0-paths, will be shortest among all paths joining its end nodes.
- 2. For e = 1, ..., k, and for $d = -\min\{e, x\}, ..., y$, do:
 - 2.1. Consider the (e-1)-paths, if any, determined in the previous step on those of diagonals d-1, d, and d+1 that exist. Each of these paths corresponds to an optimal edit script for transforming a prefix of X into a substring of Y. If possible, extend these scripts, respectively by adding an insertion, a substitution, and a deletion, thereby creating e-paths that end on diagonal d.

2.2. Of the e-paths created in step 2.1, if any, pick the one that ends farthest down diagonal d and extend it further by computing the largest common prefix of what remains of X and what remains of Y. The result will be an e-path that starts in row 0 and ends on diagonal d at the farthest possible node, being in addition shortest among all paths starting and ending at the same nodes.

The lower bound on d in step 2 reflects the fact that diagonal -e can only be reached from row 0 by an e'-path, where $1 \le e \le e' \le k$. What the entire procedure computes is a set of directed paths departing from row 0 at several columns. Each of these directed paths is an e-path, for some e such that $0 \le e \le k$, that ends as far down in the graph as possible, and is also shortest among all paths that start and end at the same nodes. So an e-path computed by the algorithm departing from node (0,d) for $0 \le d \le y$ represents an optimal edit script for turning a prefix of X into a prefix of Y[d+1..y] with e edit operations.

The basic procedure comprising steps 1 and 2 was introduced to solve the problem of approximate pattern matching [7, 11–13], which requires all approximate occurrences of X in Y having edit distance from X of at most $k \leq y$ to be determined [14]. The solution works by selecting, after the execution of steps 1 and 2, the e-paths that end on row x for $0 \leq e \leq k$. Several other solutions to this problem exist [7, 15–20].

Note that the largest common prefixes asked for in steps 1 and 2.2 can be obtained easily if we have a means of computing the largest common prefix of any two suffixes of $X\$_1Y$, where $\$_1$ is any character that does not occur in X or Y, and $X\$_1Y$ is the string obtained by appending $\$_1$ to X, then Y to $X\$_1$. Such a means, of course, is provided by the well-known suffix tree for string $X\$_1Y\$_2$, where $\$_2$ is any character not occurring in $X\$_1Y$, ultimately needed to ensure that the tree does indeed exist. After the suffix tree is built and preprocessed, which can be achieved in O(x+y) time, any of those largest common prefixes can be found in constant time [7]. Fox approximate pattern matching, $x \le y$, so O(y) is the time it takes to handle the suffix tree initially. After that, the complexity of steps 1 and 2 is dominated by step 2, which comprises O(ky) repetitions of 2.1 and 2.2, each requiring O(1) time per repetition. The overall time is then O(ky).

The same basic procedure can also be used to solve another problem involving strings X and Y, known as the k-differences problem. Assuming $k \leq \max\{x,y\}$ to avoid trivial cases, this problem asks for the edit script to transform X into Y with the fewest possible edit operations, but no more than k [13, 21]. Clearly, no solution exists if |x-y| > k. A solution may exist otherwise, and will correspond to the e-path from (0,0) to (x,y) for which e is minimum (that is, a shortest path between the two nodes), if one exists with $e \leq k$. Adapting steps 1 and 2 to find such a path is a simple matter, as follows. In step 1, let d = 0 only. In step 2, let the range for d be from $-\min\{e,x\}$ through $\min\{e,y\}$, again reflecting the fact that it takes at least e errors to reach diagonal -e or e from (0,0). Finally, abort the iterations whenever node (x,y) is reached.

This solution to the k-differences problem requires a number of matching extensions (steps 1 and 2.2) given by $1+\sum_{e=1}^k O(e)=O(k^2)$, each one requiring O(1) time after the initial construction

and preprocessing of the suffix tree for $X\$_1Y\$_2$ in O(x+y) time. The overall time is then $O(k^2+x+y)$.

This algorithm for the k-differences problem can be used directly to solve our problem of determining all maximal approximate palindromes in S, because what is required of an approximate palindrome is precisely that one of its parts be transformable into the other by means of an optimal edit script comprising no more than k edit operations. For $1 \le c \le n$, we simply let $X = S_\ell^c$ and $Y = S_r^c$ (then x + y = n or x + y = n - 1, respectively for even and odd palindromes). Whenever a new path is determined in step 2.2, we check if it is better than the ones found previously in terms of approximate-palindrome maximality; it will be better if it leads to a node whose coordinates add to a larger integer than the current best path (checking for the same integer but fewer errors is needless, as the algorithm generates shortest e-paths in nondecreasing order of e).

Apart from the time needed to establish the suffix tree for $S_{\ell}^{c}\$_{1}S_{r}^{c}\$_{2}$, this algorithm requires $O(k^{2})$ time to determine a maximal approximate palindrome in S for fixed c. Determining all even and odd approximate palindromes in S then requires $O(k^{2}n)$ time beyond what is needed to establish the suffix trees. If such a tree had indeed to be constructed and preprocessed for each c, then an additional $O(n^{2})$ time would be required. However, note that every suffix of S_{ℓ}^{c} is also a suffix of S, and that every suffix of S_{r}^{c} is also a suffix of S. So all that is required by steps 1 and 2.2, regardless of the value of c, is that a preprocessed suffix tree be available for $S^{R}\$_{1}S\$_{2}$. This tree needs to be established only once, which can be done in O(n) time, and therefore the overall complexity of determining all even and odd maximal approximate palindromes in S remains $O(k^{2}n)$.

Assessing the space required by the algorithm depends on whether edit scripts are also needed or simply the palindromes with the corresponding edit distances. In the former case, the space required for each of the O(k) diagonals is O(k); it is constant in the latter case. This, combined with the O(n) space needed for preprocessing, yields a space requirement of $O(k^2 + n)$ or O(k + n), respectively.

4. Practical improvements

Of the 2n maximal approximate palindromes determined by the algorithm of Section 3 for $c=1,\ldots,n$, three are trivial and can be skipped in a practical implementation. These are the odd palindrome for c=1, and the even and odd palindromes for c=n. For these palindromes, the optimal edit scripts contain k insertions for c=1 and k deletions for c=n. Henceforth in the paper, we then assume that the algorithm is run for $c=1,\ldots,n-1$ in the even case, $c=2,\ldots,n-1$ in the odd case.

In addition to this simplification, the algorithm introduced in Section 3 for the computation of all maximal approximate palindromes in S can be improved by selecting the range for d in step 2 more carefully. We discuss two such improvements in this section. Although they do not lead to a better execution time in the asymptotic, worst-case sense, they do bring about a reduction in execution times in practice, as we demonstrate.

The first improvement consists of skipping the diagonals on which e-paths, for suitable e, have been determined that end on row x or column y. The reason why this is safe to do is that no further path can be found ending on those diagonals farther down from row x or column y. The way to efficiently handle this improved selection of diagonals in step 2 is to keep all diagonals that are going to be processed in a doubly-linked list. This allows new diagonals to be added at the list's extremes in constant time, and diagonals that will no longer be processed can be deleted equally efficiently as soon as it is detected that the corresponding e-paths have reached the farthest row or column.

The second improvement that we describe is itself an improvement over the first one. The rationale is that, if a diagonal d is dropped from further consideration because the e-path that ends on it farthest down the grid touches, say, row x, then all other diagonals d' such that d' < d may be dropped as well. Similarly if that e-path on d touches column y, in which case not only diagonal d but also all diagonals d' such that d' > d may be dropped from further processing. What results from this improvement is that the algorithm's operation is always confined to within a strip of contiguous diagonals. This strip is limited on the left by either the leftmost diagonal on which the farthest-reaching e-path does not touch row x or diagonal $-\min\{e,x\}$; on the right, it is limited by either the rightmost diagonal on which the farthest-reaching e-path does not touch column y or diagonal $\min\{e,y\}$. As with the first improvement, it is a simple matter to implement the second one efficiently by using the same doubly-linked list.

We show in Figures 3 and 4 the gain that the first improvement elicits for a number of strings, in Figures 5 and 6 the gain due to the second improvement, and in Figures 7 and 8 the gain caused by the second improvement over the first. For Figures 3 through 6, if t_o is the the number of iterations performed by the original algorithm and t_i the number of iterations performed by the improved algorithm, then gain is defined as $(t_o - t_i)/t_o$. An iteration is either the initial execution of step 1 or each combined execution of steps 2.1 and 2.2. Because every iteration can be carried out in constant time, our assessment of gain in terms of numbers of iterations as opposed to elapsed time provides a platform-independent evaluation of the improved algorithms. Gain is defined similarly for Figures 7 and 8.

The strings we have used are the ones given next. Of these, some are *periodic*, meaning that there exists a string P of size $s \leq n$ such that the periodic string is a prefix of the string formed by concatenating $\lceil n/s \rceil$ copies of P. The *period* of the periodic string is the value of s.

- dna: A DNA sequence with n bases.
- dnap1: A periodic DNA sequence with n bases and period $\lfloor 0.05n \rfloor$.
- dnap2: A periodic DNA sequence with n bases and period |0.25n|.
- dnap3: A periodic DNA sequence with n bases and period [0.5n].
- txt: A sequence of n ASCII characters.
- txtp1: A periodic sequence of n ASCII characters with period $\lfloor 0.05n \rfloor$.

- txtp2: A periodic sequence of n ASCII characters with period |0.25n|.
- txtp3: A periodic sequence of n ASCII characters with period |0.5n|.
- *cnst*: An *n*-fold repetition of the same character.
- diff: A string comprising n different characters. This string does not fit the fixed-alphabet assumption we have made from the start, so the complexity figures given in Section 3 do not apply to executions of the algorithm on it.

Figures 3, 5, and 7 are given for n = 50, while Figures 4, 6, and 8 are for n = 2500. In each figure, the values of k, the maximum number of errors to be allowed in the approximate palindromes, are in $\{ \lceil 0.01n \rceil, \lceil 0.05n \rceil, \lceil 0.1n \rceil, \lceil 0.2n \rceil, \lceil 0.4n \rceil, \lceil 0.8n \rceil \}$. Note, in Figures 3, 5, and 7, that gains are identical for dnap1 and txtp1, owing to the fact that, for n = 50, these two strings are essentially the same, being periodic with period 2, therefore having only 2 different characters throughout.

With the single exception of Figure 7, we see in all cases that gains are largest for cnst, which can be easily accounted for by the fact that, for such a string, every diagonal is dropped from further consideration by any of the two improvements right after having been processed for the first time. The exception of Figure 7 can be explained by the fact that this figure gives gains of one improvement over the other, and together with Figure 8 gives a measure for how efficiently the second improvement creates the diagonal strips. What Figure 7 indicates is that such an efficiency is higher for dnap1 and txtp1 than it is for cnst if n = 50 and $k \ge 3$.

By contrast, gains are always smallest for *diff*, because matchings never occur in the edit scripts and therefore more iterations are needed before paths reach the grid's borders. For *diff* strings, it also happens that the second improvement provides no gain over the first.

Gains tend to be larger for sequences on smaller alphabets, because in these cases there tend to be more matchings. This is what happens for DNA sequences, which have an alphabet of size 4, therefore smaller than the alphabets of nearly all the other strings under consideration. Gains also tend to be larger as k gets larger, which is probably related to the fact that the overall number of iterations also increases with k. To finalize, we note that gains tend to decrease as n is increased, which can be seen by comparing Figures 3, 5, and 7 to Figures 4, 6, and 8, respectively. This is due to the fact that, as n gets larger, so does the number of matchings needed for paths to reach the grid's bottommost or rightmost border.

5. Expected gains

As we know from the results in Section 4, one of the key factors affecting the performance of practical implementations of our algorithm is the size of the alphabet Σ , which henceforth we let be such that $\sigma = |\Sigma|$. We discuss, in this section, a stochastic model that can be used to assess, to a limited extent, the expected gain provided by the two improvements of Section 4 for a given value of σ . The model has great richness of detail [22], and may require considerable computational effort to be solved even for strings comprising as small a number of characters as a few tens. It is

therefore not practical, but we present an outline of it nonetheless because, already for a modest range of parameters, it is capable of conveying useful information.

For fixed c, the model views an execution of the algorithm (as introduced originally or in one of its two improved variants), as a discrete-time, discrete-state stochastic process. Each time step in this stochastic process corresponds to one of the iterations on e in step 2 of the algorithm. Each state is a (2k+1)-tuple with one entry for each of the possible diagonals from -k through k. An entry contains the number of the row to which the corresponding diagonal has been stretched so far by the algorithm. The initial state has 0 in all entries.

This stochastic process never returns to a previously visited state, and can as such be represented by an acyclic directed graph whose nodes stand for states and whose directed edges represent the possible transitions among states. In this graph, every state is on some directed path from the initial state. Associated with an edge (P,Q) are two quantities, namely the probability p(P,Q) of moving from state P to state Q, and the number of diagonals to be processed when that transition is undertaken. This number of diagonals is, for each value of e, the number of iterations used in Section 4 to evaluate the two improvements as a platform-independent measure of time. It depends on whether the original algorithm or one of its two improved variants is in use, and is denoted by t(P,Q).

The crucial issue in setting up this stochastic model is of course the determination of p(P,Q) for all edges (P,Q). As it turns out, such probabilities depend on how state P is reached from the initial state, and therefore it is best to assess them dynamically as the graph is processed during the computation of one of the stochastic process' characteristics. The characteristic that interests us in this section is the expected (average) number of iterations, denoted by \bar{t} , for the algorithm to be completed on a string, n and σ being fixed in addition to c.

The following recursive procedure is a variation of straightforward depth-first traversal, and can be used to compute \bar{t} . It is started by executing step 1 on the initial state; upon termination, its output is assigned to \bar{t} .

- 1. Let P be the current state. If no edges outgo from P in the graph, then return 0. Otherwise, for z > 0, let $Q_1 \ldots, Q_z$ be the states to which a directed edge outgoes from P. Do:
 - 1.1. For i = 1, ..., z, recursively execute step 1 on state Q_i , and let t_i be its output.
 - 1.2. For i = 1, ..., z, assess the transition probability $p(P, Q_i)$ as a function of the directed path through which P was reached.
 - 1.3. Return $\sum_{i=1}^{z} (t(P,Q_i) + t_i) p(P,Q_i)$.

What remains to be presented before we discuss some results is, naturally, how to perform step 1.2 of this procedure. First we set up two matrices, called M(P) and $M(Q_i)$, representing respectively the relationships (equality, inequality, or none) that must exist between characters of two generic strings S_{ℓ}^c and S_r^c for state P to be reached from the initial state on the specific path that is being considered, and for Q_i to be reached on that same path elongated by the edge

 (P, Q_i) . If a stands for the number of different strings S satisfying the constraints of M(P) and b the number of those that satisfy the constraints of $M(Q_i)$, then $p(P, Q_i) = b/a$.

The computation of a and b can be reduced to a complex combinatorial problem, of which we give an outline next, and constitutes the computationally hardest part of the entire procedure to compute \bar{t} . Suppose we wish to compute a from M(P). The way to proceed is to start by setting up an undirected graph, call it G, whose nodes represent groups of positions in the two parts of S that by M(P) must contain the same character. Two nodes are connected by an edge if the corresponding groups of positions must, again by M(P), contain characters that differ from one group to the other. The value of a is then the number of distinct ways in which we can assign characters from Σ to the nodes of G in such a way that nodes that are connected by an edge receive different characters. This is a graph coloring problem, that is, a problem related to assigning objects (colors) to the nodes of a graph so that nodes that are connected by an edge receive different objects. The problem is to find out the number of ways in which G's nodes can be colored by a total of σ distinct colors. This number is given by the so-called chromatic polynomial of G evaluated at σ [23].

Finally, we present some numerical results. These are illustrated in Figures 9 through 12. Of these, Figures 9 and 11 are for k = 1 (n and σ vary), while Figures 10 and 12 are for n = 10 (k and σ vary). What the figures depict are the gains, averaged over c for both even and odd palindromes, that correspond to the expected times \bar{t} assessed for the original algorithm and its two variants. Figures 9 and 10 give gains for the first improvement, and Figures 11 and 12 for the second. These figures tend to support the conclusions we drew from specific examples in Section 4. These are that gains are expected to be larger for larger k and smaller σ , and smaller for larger n.

6. Concluding remarks

We have in this paper introduced a novel definition of approximate palindromes in strings, and have given an algorithm for finding all approximate palindromes in a string of n characters to within at most k errors. For a fixed alphabet, the algorithm runs in time $O(k^2n)$. We have also indicated how to perform implementation-related improvements in the algorithm, and demonstrated, over a variety of strings and also based on an average-case analysis, that such improvements do indeed often lead to reduced running times in practice.

Acknowledgments

The authors have received partial support from the Brazilian agencies CNPq and CAPES, the PRONEX initiative of Brazil's MCT under contract 41.96.0857.00, and a FAPERJ BBP grant.

References

1. D. E. Knuth, J. H. Morris, and V. R. Pratt, "Fast pattern matching in strings," SIAM J. on Computing 6 (1977), 322–350.

- 2. G. Manacher, "A new linear-time on-line algorithm for finding the smallest initial palindrome of a string," J. of the ACM 22 (1975), 346–351.
- A. Apostolico, D. Breslauer, and Z. Galil, "Optimal parallel algorithms for periods, palindromes and squares," Proc. of the Int. Colloq. on Automata, Languages, and Programming, 296–307, 1992.
- 4. A. Apostolico, D. Breslauer, and Z. Galil, "Parallel detection of all palindromes in a string," *Theoretical Computer Science* **141** (1995), 163–173.
- 5. D. Breslauer and Z. Galil, "Finding all periods and initial palindromes of a string in parallel," *Algorithmica* **14** (1995), 355–366.
- Z. Galil, "Optimal parallel algorithms for string matching," Information and Control 67 (1985), 144–157.
- 7. D. Gusfield, Algorithms on Strings, Trees, and Sequences: Computer Science and Computational Biology, Cambridge University Press, New York, NY, 1997.
- 8. J. Jurka, "Origin and evolution of Alu repetitive elements," in R. J. Maraia (Ed.), *The Impact of Short Interspersed Elements (SINEs) on the Host Genome*, R. G. Landes, New York, NY, 25–41, 1995.
- 9. V. I. Levenstein, "Binary codes capable of correcting insertions and reversals," *Soviet Physics Doklady* **10** (1966), 707–710.
- D. Sankoff and J. Kruskal (Eds.), Time Warps, String Edits, and Macromolecules: The Theory and Practice of Sequence Comparison, Addison-Wesley, Reading, MA, 1983.
- 11. G. M. Landau and U. Vishkin, "Introducing efficient parallelism into approximate string matching and a new serial algorithm," *Proc. of the Annual ACM Symp. on Theory of Computing*, 220–230, 1986.
- 12. G. M. Landau and U. Vishkin, "Fast parallel and serial approximate string matching," *J. of Algorithms* **10** (1989), 157–169.
- 13. E. W. Myers, "An O(nd) difference algorithm and its variations," Algorithmica 1 (1986), 251-266.
- 14. E. Ukkonen, "Algorithms for approximate string matching," *Information and Control* **64** (1985), 100–118.
- 15. R. Baeza-Yates and G. Navarro, "Faster approximate string matching," *Algorithmica* **23** (1999), 127–158.
- 16. W. I. Chang and J. Lampe, "Theoretical and empirical comparisons of approximate string matching algorithms," *Proc. of the Symp. on Combinatorial Pattern Matching*, 175–184, 1992.

- 17. R. Cole and R. Hariharan, "Approximate string matching: a simpler faster algorithm," *Proc.* of the Annual ACM-SIAM Symp. on Discrete Algorithms, 463–472, 1998.
- 18. G. A. Stephen, String Searching Algorithms, World Scientific, Singapore, 1994.
- 19. E. Ukkonen, "Finding approximate patterns in strings," J. of Algorithms 6 (1985), 132–137.
- 20. S. Wu and U. Manber, "Fast text searching allowing errors," Comm. of the ACM **35** (1992), 83–91.
- 21. G. M. Landau and U. Vishkin, "Efficient string matching with k mismatches," *Theoretical Computer Science* **43** (1986), 239–249.
- 22. A. H. L. Porto, *Detecting Approximate Palindromes in Strings*, M.Sc. Thesis, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, 1999 (in Portuguese).
- J. A. Bondy and U. S. R. Murty, Graph Theory with Applications, North-Holland, New York, NY, 1976.

Authors' biographical data

Alexandre H. L. Porto is a doctoral student at the Systems Engineering and Computer Science Program of the Federal University of Rio de Janeiro. He is interested in sequential and parallel algorithms for problems in computational biology.

Valmir C. Barbosa is professor at the Systems Engineering and Computer Science Program of the Federal University of Rio de Janeiro, and is interested in the various aspects of distributed and parallel computing, as well as of the so-called complex systems, like neural networks and related models. He received his Ph.D. from the University of California, Los Angeles, in 1986, and has held visiting positions at the IBM Rio Scientific Center in Brazil, the International Computer Science Institute in Berkeley, and the Computer Science Division of the University of California, Berkeley. He has authored the books Massively Parallel Models of Computation (Ellis Horwood, Chichester, UK, 1993), An Introduction to Distributed Algorithms (The MIT Press, Cambridge, MA, 1996), and An Atlas of Edge-Reversal Dynamics (Chapman & Hall/CRC Press, London, UK, 2000).

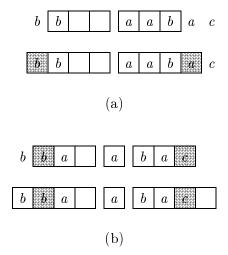


Figure 1. Even (a) and odd (b) approximate palindromes for k=3 in the string bbaabac

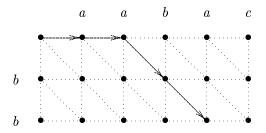


Figure 2. An edit script as a directed path in D

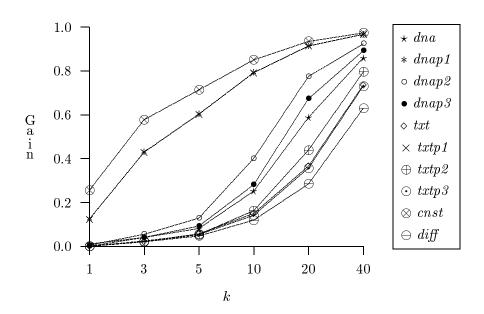


Figure 3. Gains due to the first improvement for n = 50

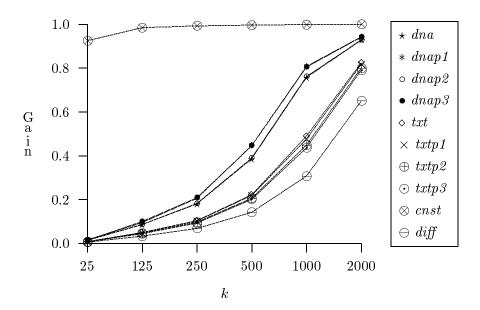


Figure 4. Gains due to the first improvement for n=2500

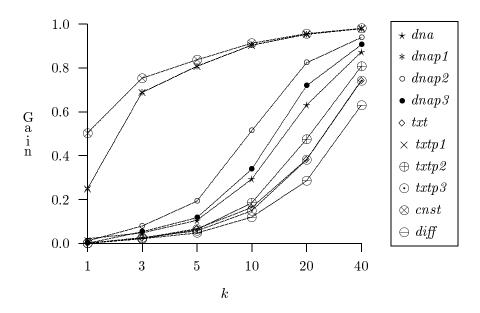


Figure 5. Gains due to the second improvement for n = 50

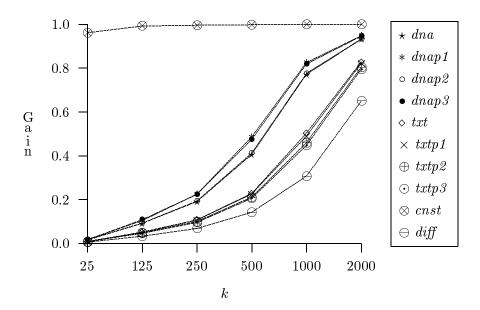


Figure 6. Gains due to the second improvement for n = 2500

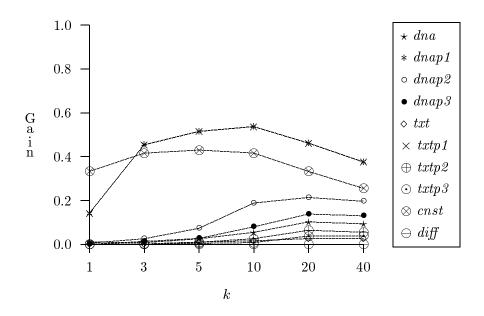


Figure 7. Gains of the second improvement over the first for n = 50

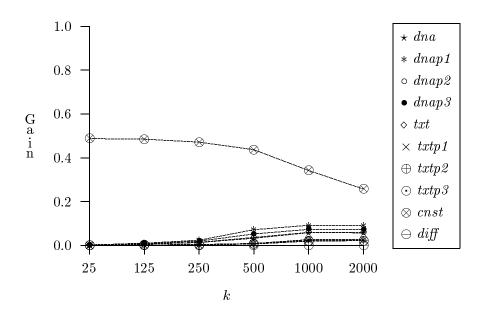


Figure 8. Gains of the second improvement over the first for n=2500

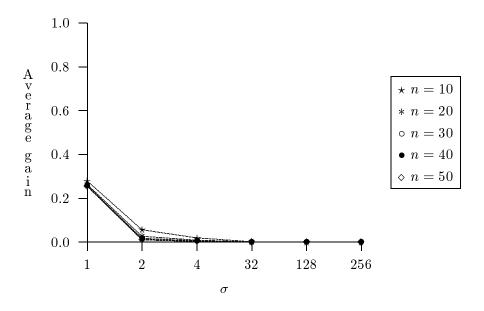


Figure 9. Average gains due to the first improvement for k=1

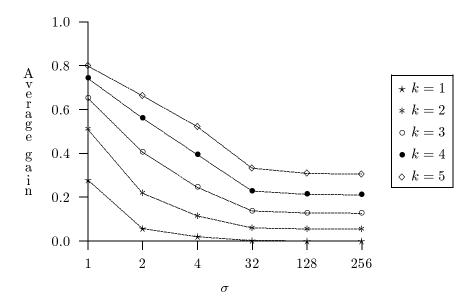


Figure 10. Average gains due to the first improvement for n = 10

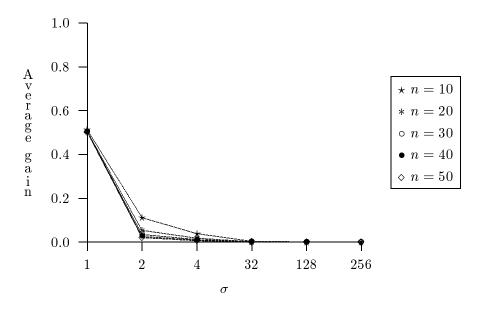


Figure 11. Average gains due to the second improvement for k=1

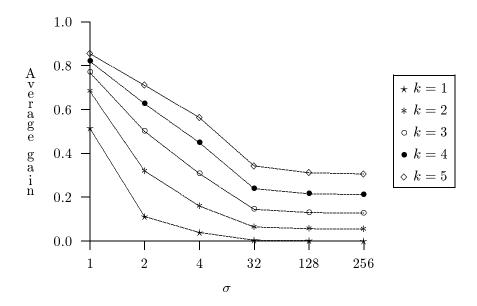


Figure 12. Average gains due to the second improvement for n = 10