On string matching with k mismatches

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Abstract—In this paper we consider several variants of the pattern matching problem. In particular, we investigate the following problems: 1) Pattern matching with k mismatches; 2) Approximate counting of mismatches; and 3) Pattern matching with mismatches. The distance metric used is the Hamming distance. We present some novel algorithms and techniques for solving these problems. Both deterministic and randomized algorithms are offered. Variants of these problems where there could be wild cards in either the text or the pattern or both are considered. An experimental evaluation of these algorithms is also presented. The source code is available at http://www.engr.uconn.edu/~man09004/kmis.zip

Index Terms—pattern matching with mismatches, k mismatches problem, approximate string matching

1 INTRODUCTION

The problem of string matching has been studied extensively due to its wide range of applications from Internet searches to computational biology. The simplest version takes as input a text $T = t_1 t_2 \cdots t_n$ and a pattern $P = p_1 p_2 \cdots p_m$ from an alphabet $\Sigma$. The problem is to find all the occurrences of the pattern in the text. Algorithms for solving this problem in $O(n + m)$ time are well known (e.g., [1]). A variation of this problem searches for multiple patterns at the same time (e.g., [2]). A more general version allows for “don’t care” or “wild card” characters (they match any character) in the text and the pattern. A simple $O(n \log |\Sigma| \log m)$ algorithm for pattern matching with wild cards is given in [3]. A randomized $O(n \log n)$ algorithm which solves the problem with high probability is given in [4]. A slightly faster randomized $O(n \log m)$ algorithm is given in [5]. A simple deterministic $O(n \log m)$ algorithm based on convolutions is given in [6].

A more challenging instance of the problem is pattern matching with mismatches. There are two versions: a) for every alignment of the pattern in the text, find the distance between the pattern and the text, or b) identify only those alignments where the distance between the pattern and the text is less than a given threshold. The distance metric can be the Hamming distance, edit distance, L1 metric, and so on. In [7] the problem has been generalized to use trees instead of sequences or to use sets of characters instead of single characters. The Hamming distance between two strings of equal length is defined as the number of positions where the two strings differ. In this paper we are interested in the following two problems, with and without wild cards.

1.1 Pattern matching with mismatches

For pattern matching with mismatches, the naive algorithm computes the Hamming distance for every alignment of the pattern in the text, in time $O(nm)$. A faster algorithm is Abrahamson’s algorithm, which runs in time $O(n \sqrt{m \log m})$. We prove that this algorithm can be modified to obtain an $O(n \sqrt{g \log m})$ time algorithm for pattern matching with mismatches and wild cards, where $g$ is the number of non-wild card positions in the pattern. This gives a simpler and faster alternative to an algorithm proposed in [8].

In the literature, we also find algorithms which approximate the number of mismatches for every alignment. For example, [9] gives an $O(r n \log m)$ time algorithm for pattern matching with mismatches, in the absence of wild cards, where $r$ is the number of iterations of the algorithm. Every distance reported has a variance bounded by $(m - c_i)/r^2$ where $c_i$ is the exact number of matches for alignment $i$. [10] gives an $O(n \log^2 m/\epsilon^2)$ time randomized algorithm which approximates the Hamming distance for every alignment within an $\epsilon$ factor, in the absence of wild cards. We show how to extend this algorithm to pattern matching with mismatches and wild cards. The new algorithm approximates the Hamming distance for every alignment within an $\epsilon$ factor in time $O(n \log^2 m/\epsilon^2)$ with high probability.
1.2 Pattern matching with \( k \) mismatches

For the \( k \)-mismatches problem, without wild cards, \( O(nk) \) time algorithms are presented in \cite{11}, \cite{12}. A faster \( O(n\sqrt{k\log k}) \) time algorithm is presented in \cite{8}. This algorithm combines the two main techniques known in the literature for pattern matching with mismatches: filtering and convolutions. We give a significantly simpler algorithm having the same worst case run time. Furthermore, the new algorithm will never perform more operations than the one in \cite{8} during marking and convolution.

An intermediate problem is to check if the Hamming distance is less or equal to \( k \) for a subset of the aligned positions. This problem can be solved with the Kangaroo method proposed in \cite{8} at a cost of \( O(k) \) time per alignment, using \( O(n + m) \) additional memory. We show how to achieve the same run time per alignment using only \( O(m) \) additional memory.

Further, we look at the version of \( k \)-mismatches where wild cards are allowed in the text and the pattern. For this problem, two randomized algorithms are presented in \cite{13}. The first one runs in \( O(nk \log n \log m) \) time and the second one in \( O(n \log m (k + \log n \log \log n)) \) time. Both are Monte Carlo algorithms, i.e., they output the correct answer with high probability. The same paper also gives a deterministic algorithm with a run time of \( O(nk^2 \log^2 m) \). Also, a deterministic \( O(nk^2 \log^2 m (\log^2 k + \log \log m)) \) time algorithm is given in \cite{14}. We present a Las Vegas algorithm (that always outputs the correct answer) which runs in time \( O(nk \log^2 m + n \log^2 m \log n + n \log m \log n \log \log n) \) with high probability.

The contributions of this paper can be summarized as follows.

For pattern matching with mismatches:

- An \( O(n\sqrt{g \log m}) \) time algorithm for pattern matching with mismatches and wild cards, where \( g \) is the number of non-wild card positions in the pattern.
- A randomized algorithm that approximates the Hamming distance for every alignment, when wild cards are present, within an \( \epsilon \) factor in time \( O(n \log^2 m/\epsilon^2) \) with high probability.

For pattern matching with \( k \) mismatches:

- An \( O(n \sqrt{k \log k}) \) time algorithm for pattern matching with \( k \) mismatches, without wild cards, which is simpler and has a better expected run time than the one in \cite{8}.
- An algorithm that tests if the Hamming distance is less than \( k \) for a subset of the alignments, without wild cards, at a cost of \( O(k) \) time per alignment, using only \( O(m) \) additional memory.
- A Las Vegas algorithm for the \( k \)-mismatches problem with wild cards that runs in time \( O(nk \log^2 m + n \log^2 m \log n + n \log m \log n \log \log n) \) with high probability.

The rest of the paper is organized as follows. First we introduce some notations and definitions. Then we present the randomized and approximate algorithms: first the Las Vegas algorithm for \( k \)-mismatches with wild cards, then the algorithm for approximate counting of mismatches in the presence of wild cards. Then we describe the deterministic and exact algorithms, for which we also present an empirical run time comparison.

2 Some definitions

Given two strings \( T = t_1 t_2 \ldots t_n \) and \( P = p_1 p_2 \ldots p_m \) (with \( m \leq n \)), the convolution of \( T \) and \( P \) is a sequence \( C = c_1, c_2, \ldots, c_{n-m+1} \) where \( c_i = \sum_{j=1}^{m} t_{i+j-1} p_j \), for \( 1 \leq i \leq (n-m+1) \). We can compute this convolution in \( O(n \log m) \) time using the Fast Fourier Transform. Some speedup techniques exist \cite{15} for convolutions applied on binary inputs, as is usually the case with pattern matching.

In the context of randomized algorithms, by high probability we mean a probability greater or equal to \((1 - \epsilon)\alpha\) where \( n \) is the input size and \( \alpha \) is a probability parameter usually assumed to be a constant greater than 0. The run time of a Las Vegas algorithm is said to be \( O(f(n)) \) if the run time is no more than \( c \alpha f(n) \) with probability greater or equal to \((1 - \epsilon)\alpha\) for all \( n \geq n_0 \), where \( c \) and \( n_0 \) are some constants, and for any constant \( \alpha \geq 1 \).

3 A Las Vegas algorithm for \( k \)-mismatches

3.1 The 1-Mismatch Problem

Problem Definition: For this problem also, the input are two strings \( T \) and \( P \) with \( |T| = n, |P| = m, \) and \( m \leq n \). Let \( T_i \) stand for the substring \( t_i t_{i+1} \ldots t_{i+m-1} \), for any \( i \), with \( 1 \leq i \leq (n-m+1) \). The problem is to check if the Hamming distance between \( T_i \) and \( P \) is exactly 1, for any \( i \). The following Lemma is shown in \cite{13}.

**Lemma 1:** The 1-mismatch problem can be solved in \( O(n \log m) \) time using a constant number of convolution operations.

The Algorithm: Assume that each wild card in the pattern as well as the text is replaced with a zero. Also, assume that the characters in the text as well as the pattern are integers in the range \([1 : \Sigma]\) where \( \Sigma \) is the alphabet under concern. Let \( e_{i,j} \) stand for the “error term” introduced by the character \( t_{i+j-1} \) in \( T_i \) and the character \( p_j \) in \( P \) and its value is \((t_{i+j-1} - p_j)^2 t_{i+j-1} p_j \). Also, let \( E_i = \sum_{j=1}^{m} e_{i,j} \). There are four steps in the algorithm:

1) Compute \( E_i \) for \( 1 \leq i \leq (n-m+1) \). Note that \( E_i \) will be zero if \( T_i \) and \( P \) match (assuming that a wild card can be matched with any character).
2) Compute \( E'_i \) for \( 1 \leq i \leq (n-m+1) \), where \( E'_i = \sum_{j=1}^{m} (i+j-1)(t_{i+j-1} - p_j)^2 p_j t_{i+j-1} \) (for \( 1 \leq i \leq (n-m+1) \)).
3) Let $B_i = E_i / E_i$ if $E_i \neq 0$, for $1 \leq i \leq (n - m + 1)$. Note that if the Hamming distance between $T_i$ and $P$ is exactly one, then $B_i$ will give the position in the text where this mismatch occurs.

4) If for any $i$ ($1 \leq i \leq (n - m + 1)$), $E_i \neq 0$ and if $(t(B_i) - p_{B_i - i + 1})^2 t(B_i) p_{B_i - i + 1} = E_i$ then we conclude that the Hamming distance between $T_i$ and $P$ is exactly one.

**Note:** If the Hamming distance between $T_i$ and $P$ is exactly 1 (for any $i$), then the above algorithm will not only detect it but also identify the position where there is a mismatch. Specifically, it will identify the integer $j$ such that $t_{i+j-1} \neq p_j$.

### 3.2 The Randomized Algorithms of [13]

Two different randomized algorithms are presented in [13] for solving the $k$-mismatch problem. Both are Monte Carlo algorithms. In particular, they output the correct answers with high probability. The run times of these algorithms are $O(nk \log m \log n)$ and $O(n \log m (k + \log n \log \log n))$, respectively. In this section we provide a summary of these algorithms.

The first algorithm has $O(k \log n)$ sampling phases and in each phase a 1-mismatch problem is solved. Each phase of sampling works as follows. We choose $m/k$ positions of the pattern uniformly at random. The pattern $P$ is replaced by a string $P'$ where $|P'| = m$, the characters in $P'$ in the randomly chosen positions are the same as those in the corresponding positions of $P$, and the rest of the characters in $P'$ are chosen to be wild cards. The 1-mismatch algorithm of Lemma 1 is run on $T$ and $P'$. In each phase of random sampling, for each $i$, we get to know if the Hamming distance between $T_i$ and $P'$ is exactly 1 and, if so, identify the $j$ such that $t_{i+j-1} \neq p_{j}'$.

As an example, consider the case when the Hamming distance between $T_i$ and $P$ is $k$ (for some $i$). Then, in each phase of sampling we would expect to identify exactly one of the positions (i.e., $j$) where $T_i$ and $P$ differ (i.e., $t_{i+j-1} \neq p_{j}$). As a result, in an expected $k$ phases of sampling we will be able to identify all the $k$ positions in which $T_i$ and $P$ differ. It can be shown that if we make $O(k \log n)$ sampling phases, then we can identify all the $k$ mismatches with high probability [13].

Let the number of mismatches between $T_i$ and $P$ be $q_i$ (for $1 \leq i \leq (n - m + 1)$). If $q_i \leq k$, the algorithm of [13] will compute $q_i$ exactly. If $q_i > k$, then the algorithm will report that the number of mismatches is $> k$ (without estimating $q_i$) and this answer will be correct with high probability. The algorithm starts off by first computing $E_i$ values for every $T_i$. A list $L(i)$ of all the mismatches found for $T_i$ is kept, for every $i$. Whenever a mismatch is found between $T_i$ and $P$ (say in position $(i + j - 1)$ of the text), the value of $E_i$ is reduced by $e_{i,j}$. If at any point in the algorithm $E_i$ becomes zero for any $i$ it means that we have found all the $q_i$ mismatches between $T_i$ and $P$ and $L(i)$ will have the positions in the text where these mismatches occur. Note that if the Hamming distance between $T_i$ and $P$ is much larger than $k$ (for example close or equal to $m$), then the probability that in a random sample we isolate a single mismatch is very low. Therefore, if the number of sample phases is only $O(k \log n)$, the algorithm can only be Monte Carlo. Even if $q_i \leq k$, there is a small probability that we may not be able to find all the $q_i$ mismatches. Call this algorithm Algorithm 1. If for each $i$, we either get all the $q_i$ mismatches (and hence the corresponding $E_i$ is zero) or we have found $> k$ mismatches between $T_i$ and $P$ then we can be sure that we have found all the correct answers (and the algorithm will become Las Vegas).

The authors of [13] also present an improved algorithm whose run time is $O(n \log m (k + \log n \log \log n))$. The main idea is the observation that if $q_i = k$ for any $i$, then in $O(k \log n)$ sampling steps we can identify $\geq k/2$ mismatches. There are several iterations where in each iteration $O(k + \log n)$ sampling phases are done. At the end of each iteration the value of $k$ is changed to $k/2$. Let this algorithm be called Algorithm 2.

### 3.3 A Las Vegas Algorithm

In this section we present a Las Vegas algorithm for the $k$-mismatches problem when there are wild cards in the text and/or the pattern. This algorithm runs in time $O(nk \log^2 m + n \log^2 m \log n + n \log m \log n \log \log n)$. This algorithm is based on the algorithm of [13]. When the algorithm terminates, for each $i$ ($1 \leq i \leq (n - m + 1)$), either we would have identified all the $q_i$ mismatches between $T_i$ and $P$ or we would have identified more than $k$ mismatches between $T_i$ and $P$.

Algorithm 1 will be used for every $i$ for which $q_i \leq 2k$. For every $i$ for which $q_i > 2k$ we use the following strategy. Let $2^\ell < q_i \leq 2^{\ell+1}k$ (where $1 \leq \ell \leq \log \left(\frac{n}{\log^2 m}\right)$). Let $w = \log \left(\frac{m}{2^{\ell+1}k}\right)$. There will be $w$ phases in the algorithm and in each phase we perform $O(k)$ sampling steps. Each sampling step in phase $\ell$ involves choosing $\frac{m}{2^{\ell+1}k}$ positions of the pattern uniformly at random (for $1 \leq \ell \leq w$). As we show below, if for any $i$, $q_i$ is in the interval $[2^\ell, 2^{\ell+1}]$, then at least $k$ mismatches between $T_i$ and $P$ will be found in phase $\ell$ with high probability. A pseudocode for the algorithm (call it Algorithm 3) is given below. An analysis will follow.

**Algorithm 3**

repeat

1. Run Algorithm 1 or Algorithm 2
2. for $\ell := 1$ to $w$ do
   for $r := 1$ to $ck$ (being a constant) do
     Uniformly randomly choose $\frac{m}{2^{\ell+1}k}$ positions of the pattern;

Generate a string $P'$ such that $|P'| = |P|$ and $P'$ has the same characters as $P$ in these randomly chosen positions and zero everywhere else.

Run the 1-mismatch algorithm on $T$ and $P'$.

As a result, if there is a single mismatch between $T_i$ and $P'$, then add the position of mismatch to $L(i)$ and reduce the value of $E_i$ by the right amount, for $1 \leq i \leq (n-m+1)$;

3. if $E_i = 0$ or $|L(i)| > k$ for every $i$, $1 \leq i \leq (n-m+1)$ then quit;

forever

Theorem 1: Algorithm 3 runs in time $\tilde{O}(nk \log^2 m + n \log^2 m \log n + n \log m \log n \log \log n)$ if Algorithm 2 is used in step 1. It runs in time $\tilde{O}(nk \log m \log n + nk \log^2 m + n \log^2 m \log n)$ if step 1 uses Algorithm 1.

Proof: As shown in [13], the run time of Algorithm 1 is $O(nk \log m \log n)$ and that of Algorithm 2 is $O(n \log m (k + \log n \log \log n))$. The analysis will be done with respect to an arbitrary $T_i$. In particular, we will show that after the specified amount of time, with high probability, we will either know $q_i$ or realize that $q_i > k$. It will then follow that the same statement holds for every $T_i$ (for $1 \leq i \leq (n-m+1)$).

Consider phase $\ell$ of step 2 (for an arbitrary $1 \leq \ell \leq w$). Let $2^i k < q_i \leq 2^{i+1} k$ for some $i$. Using the fact that $\binom{n}{q_i} \approx \left(\frac{ae}{b}\right)^{q_i}$, the probability of isolating one of the mismatches in one run of the sampling step is:

$$\frac{(m/2^{i+1}k-1)q_i}{(m/2^{i+1}k)} \geq \frac{(m-2^{i+1}k-1)2^j k}{(m/2^{i+1}k)2^j k} \geq \frac{1}{2e}$$

As a result, using Chernoff bounds, it follows that if $13ke$ sampling steps are made in phase $\ell$, then at least $6k$ of these steps will result in the isolation of single mismatches (not all of them need be distinct) with high probability (assuming that $k = \Omega(\log n)$). Moreover, we can see that at least 1.1k of these mismatches will be distinct. This is because the probability that $\ell \leq 1.1k$ of these are distinct is $\left(\frac{n}{1.1k}\right)^{6k} = 2^{-2.64k}$ using the fact that $q_i \geq 2k$. This probability will be very low when $k = \Omega(\log n)$.

In the above analysis we have assumed that $k = \Omega(\log n)$. If this is not the case, in any phase of step 2, we can do $c \log n$ sampling steps, for some suitable constant $c$. As a result, each phase of step 2 takes $O(n \log m (k + \log n))$ time. We have $O(\log m)$ phases. Thus the run time of step 2 is $O(n \log^2 m (k + \log n))$. Also, the probability that the condition in step 3 holds is very high.

Therefore, the run time of the entire algorithm is $\tilde{O}(nk \log^2 m + n \log^2 m \log n + n \log m \log n \log \log n)$ if Algorithm 2 is used in step 1 or $\tilde{O}(nk \log m \log n + nk \log^2 m + n \log^2 m \log n)$ if Algorithm 1 is used in step 1.

4 Approximate Counting of Mismatches

The algorithm of [10] takes as input a text $T = t_1 t_2 \ldots t_n$, and a pattern $P = p_1 p_2 \ldots p_m$, and approximately counts the Hamming distance between $T_i$ and $P$ for every $1 \leq i \leq (n-m+1)$. In particular, if the Hamming distance between $T_i$ and $P$ is $H_i$ for some $i$, then the algorithm outputs $h_i$ where $H_i \leq h_i \leq (1+c)H_i$ for any $c > 0$ with high probability (i.e., a probability of $\geq (1-m^{-a})$). The run time of the algorithm is $O(n \log^2 m/c^2)$. In this section we show how to extend this algorithm to the case where there could be wild cards in the text and/or the pattern.

Let $\Sigma$ be the alphabet under concern and let $\sigma = |\Sigma|$. The algorithm runs in phases and in each phase we randomly map the elements of $\Sigma$ to $\{1, 2\}$. A wild card is mapped to a zero. Under this mapping we transform $T$ and $P$ to $T'$ and $P'$, respectively. We then compute a vector $C$ where $C[i] = \sum_{j=1}^{m} (t_{i+j-1} - p_{j-1}) h_{i+j-1} p_j$. This can be done using $O(1)$ convolution operations (see e.g., [13]). A series of $r$ such phases (for some relevant value of $r$) is done at the end of which we produce estimates on the Hamming distances. The intuition is that if a character $x$ in $T'$ is aligned with a character $y$ in $P'$, then across all the $r$ phases, the expected contribution to $C$ from these characters is $r$ if $x \neq y$ (assuming that $x$ and $y$ are non wild cards). If $x = y$ or if one or both of $x$ and $y$ are a wild card, the contribution to $C$ is zero.

Algorithm 4

1. for $i := 1$ to $(n-m+1)$ do $C[i] := 0$.
2. for $\ell := 1$ to $r$ do

Let $Q$ be a random mapping of $\Sigma$ to $\{1, 2\}$. In particular, each element of $\Sigma$ is mapped to 1 or 2 randomly with equal probability. Each wild card is mapped to a zero. Obtain two strings $T'$ and $P'$ where $t'_i = Q(t_i)$ for $1 \leq i \leq n$ and $p'_j = Q(p_j)$ for $1 \leq j \leq m$. Compute a vector $C_{\ell}$ where $C_{\ell}[i] = \sum_{j=1}^{m} (t'_{i+j-1} - p'_{j-1})^2 t'_{i+j-1} p'_j$ for $1 \leq i \leq (n-m+1)$.

for $i := 1$ to $(n-m+1)$ do $C[i] := C[i] + C_{\ell}[i]$.
3. for $i := 1$ to $(n-m+1)$ do

output $h_i := \frac{C[i]}{r}$.

Here $h_i$ is an estimate on the Hamming distance $H_i$ between $T_i$ and $P$.

Analysis: Let $x$ be a character in $T$ and let $y$ be a character in $P$. Clearly, if $x = y$ or if one or both of $x$ and $y$ are a wild card, the contribution of $x$ and $y$ to any $C[i]$ is zero. If $x$ and $y$ are non wild cards and if $x \neq y$ then the expected contribution of these to any $C[i]$ is 1. Across all the $r$ phases, the expected contribution of $x$ and $y$ to any $C[i]$ is $r$. For a given $x$ and $y$, we can think of each phase as a Bernoulli trial with equal probabilities for success and failure. A success refers to the possibility of $Q(x) \neq Q(y)$. 


The expected number of successes in \( r \) phases is \( \frac{r}{r} \).
Using Chernoff bounds, this contribution is no more than \( (1 + \epsilon)r \) with probability \( \geq 1 - \exp(-\epsilon^2 r/6) \).
Probability that this statement holds for every pair \((x, y)\) is \( \geq 1 - m^2 \exp(-\epsilon^2 r/6) \). This probability will be \( \geq 1 - m^{-\alpha}/2 \) if \( r \geq \frac{6(\alpha+3)\log\,m}{\epsilon^2} \). Similarly, we can show that for any pair of non-wild card characters, the contribution of them to any \( C[i] \) is no less than \( (1 - \epsilon)r \) with probability \( \geq 1 - m^{-\epsilon}/2 \) if \( r \geq \frac{6(\alpha+3)\log\,m}{\epsilon^2} \).

Put together, for any pair \((x, y)\) of non wild cards, the contribution of \( x \) and \( y \) to any \( C[i] \) is in the interval \((1 \pm \epsilon)r \) with probability \( \geq (1 - m^{-\epsilon}) \) if \( r \geq \frac{6(\alpha+3)\log\,m}{\epsilon^2} \). Let \( H_i \) be the Hamming distance between \( T_i \) and \( P \) for some \( i \) \((1 \leq i \leq (n - m + 1))\), then, the estimate \( h_i \) on \( H_i \) will be in the interval \((1 \pm \epsilon)H_i \) with probability \( \geq (1 - m^{-\epsilon}) \). As a result, we get the following Theorem.

**Theorem 2:** Given a text \( T \) and a pattern \( P \), we can estimate the Hamming distance between \( T_i \) and \( P \) for every \( i \), \( 1 \leq i \leq (n - m + 1) \), in \( O(n \log^2 m / \epsilon^2) \) time. If \( H_i \) is the Hamming distance between \( T_i \) and \( P \), then the above algorithm outputs an estimate that is in the interval \((1 \pm \epsilon)H_i \) with high probability.

**Observation 1.** In the above algorithm we can ensure that \( h_i \geq H_i \) and \( h_i \leq (1 + \epsilon)H_i \) with high probability by changing the estimate computed in step 3 of Algorithm 4 to \( \frac{C[i]}{(1 - \epsilon)r} \).

**Observation 2.** As in [8], with \( O\left(\frac{m^2 \log m}{\epsilon^2}\right) \) pre-processing we can ensure that Algorithm 4 never errs (i.e., the error bounds on the estimates will always hold).

## 5 Deterministic Algorithms

In this section we present deterministic algorithms for the problems of interest. We first summarize two well known techniques for counting matches: convolution and marking (see e.g. [8]). In terms of notation, \( T[i] \) is the character at position \( i \) in \( T \), \( T_{i,j} \) is the substring of \( T \) between \( i \) and \( j \) and \( T_i \) is \( T_{i,i+m-1} \) as before.

**Convolution:** Given a string \( S \) and a character \( \alpha \) define \( S^{\alpha} \) to be a string where \( S^{\alpha}[i] = 1 \) if \( S[i] = \alpha \) and 0 otherwise. Let \( C^{\alpha} = \text{convolution}(T^{\alpha}, P^{\alpha}) \).

Then \( C^{\alpha} \) gives the number of positions \( j \) where \( P[j] = T[i + j - 1] = \alpha \), which is the number of matches “contributed” by character \( \alpha \) to the alignment between \( P \) and \( T_i \). Then \( \sum_{\alpha \in \Sigma} C^{\alpha}[i] \) is the number of matches between \( P \) and \( T_i \).

**Marking:** Given a character \( \alpha \) let \( Pos[\alpha] = \{i \in [1..m] | P[i] = \alpha \} \).

**Algorithm 5** \( Mark(T, n, \Gamma) \)

\[
\begin{align*}
\text{for } i := 1 \text{ to } n \text{ do } M[i] := 0 \\
\text{for } i := 1 \text{ to } n, \text{ if } T[i] \in \Gamma \text{ do }
\end{align*}
\]

for \( j \in Pos[T[i]], \text{ if } i - j + 1 > 0 \) do

\[
M[i - j + 1]++
\]

return \( M \)

### 5.1 Pattern matching with mismatches

For pattern matching with mismatches, without wild cards, Abrahamson [16] gave the following \( O(n \sqrt{m \log m}) \) time algorithm. Let \( A \) be a set of the most frequent characters in the pattern. 1) Using convolutions, count how many matches each character in \( A \) contributes to every alignment. 2) Using marking, count how many matches each character in \( \Sigma - A \), contributes to every alignment. 3) Add the two numbers to find for every alignment, the number of matches between the pattern and the text. The convolutions take \( O(|A|n \log m) \) time. A character in \( \Sigma - A \) cannot appear more than \( m/|A| \) times in the pattern, otherwise, each character in \( A \) has a frequency greater than \( m/|A| \), which is not possible. Thus, the run time for marking is \( O(mn/|A|) \). If we equate the two run times we find the optimal \( |A| = \sqrt{m/\log m} \) which gives a total run time of \( O(n \sqrt{m \log m}) \).

For pattern matching with mismatches and wild cards, a fairly complex algorithm is given in [8]. The run time is \( O(n \sqrt{g \log m}) \) where \( g \) is the number of non-wild card positions in the pattern. The problem can also be solved through a simple modification of Abrahamson’s algorithm, in time \( O(n \sqrt{m \log m}) \), as pointed out in [13]. We now prove the following result:

**Theorem 3:** Pattern matching with mismatches and wild cards can be solved in \( O(n \sqrt{g \log m}) \) time, where \( g \) is the number of non-wild card positions in the pattern.

**Proof:** Ignoring the wild cards for now, let \( A \) be the set of the most frequent characters in the pattern. As above, count matches contributed by characters in \( A \) and \( \Sigma \setminus A \) using convolution and marking respectively. By a similar reasoning as above, the characters used in the marking phase will not appear more than \( g/|A| \) times in the pattern. If we equate the run times for the two phases we obtain \( O(n \sqrt{g \log m}) \).

We are now left to count how many matches are contributed by the wild cards. For a string \( S \) and a character \( \alpha \), define \( S^{\alpha} \) as \( S^{\alpha}[i] = 1 - S[i] \).

Let \( w \) be the wild card character. Compute \( C = \text{convolution}(T^{\alpha}, P^{\alpha, w}) \). Then, for every alignment \( i \), the number of positions that have a wild card either in the text or the pattern or both, is \( m - C[i] \). Add \( m - C[i] \) to the previously computed counts and output. The total run time is \( O(n \sqrt{g \log m}) \).

### 5.2 Pattern matching with \( k \) mismatches

For the \( k \)-mismatches problem, without wild cards, an \( O(k(m \log m + n)) \) time algorithm that requires \( O(k(m + n)) \) additional space is presented in [11]. Another algorithm, that takes \( O(m \log m + kn) \) time
and uses only $O(m)$ additional space is presented in [12]. We define the following problem which is of interest in the discussion.

Problem 1: Subset $k$-mismatches: Given a text $T$ of length $n$, a pattern $P$ of length $m$, a set of positions $S = \{i|1 \leq i \leq n - m + 1\}$ and an integer $k$, output the positions $i \in S$ for which the Hamming distance between $P$ and $T_i$ is less or equal to $k$.

The problem becomes the regular $k$-mismatches problem if $|S| = n$. However, if $S$ contains only a fraction of all positions, the $O(nk)$ algorithms mentioned above are too costly. A better alternative is proposed in [8]: build a suffix tree of $T \# P$ and enhance it to support LCA queries in $O(1)$ time. Given position $i$, perform an LCA query to find the position of the first mismatch between $P$ and $T_i$, call it $j$. Then, perform another LCA to find the first mismatch between $P_{j+1...m}$ and $T_{i+j+1...i+m-1}$, which is the second mismatch of alignment $i$. Repeatedly jump from one mismatch to the next, until the end of the pattern is reached or we have found more than $k$ mismatches. This is called the Kangaroo method. It can process $|S|$ positions in $O(n + m + |S|k)$ time and it uses $O(n + m)$ additional memory for the LCA enhanced suffix tree. We prove the following result:

Theorem 4: Subset $k$-mismatches can be solved in $O(n + m + |S|k)$ time using only $O(m)$ additional memory.

Proof: The algorithm is the following - also see algorithm 6 in the appendix. Build an LCA-enhanced suffix tree of the pattern. 1) Find the longest unscanned region of the text which can be found somewhere in the pattern. 2) For every alignment that overlaps this region of the text, count how many mismatches are found in the overlapping region. To do this, we compare the pattern against itself, by using LCA queries, because we know that the text is the same as the pattern, in that region. Repeat from step 1 until the entire text has been scanned. Every time we process an alignment in step 2, we either discover at least one additional mismatch or we reach the end of the alignment. This is true since in step 1 we always pick the longest portion of text that can be found somewhere in the pattern. In addition, every alignment for which we have found more than $k$ mismatches is excluded from further consideration. This ensures we spend $O(k)$ time per alignment. It takes $O(m)$ time to build the LCA enhanced suffix tree of the pattern and $O(n)$ additional time to scan the text from left to right. Thus, the total run time is $O(n + m + |S|k)$ with $O(m)$ additional memory. $\square$

5.3 An $O(n\sqrt{k\log k})$ time algorithm for $k$-mismatches

For the $k$-mismatches problem, without wild cards, a fairly complex $O(n\sqrt{k\log k})$ time algorithm is given in [8]. The algorithm classifies the inputs into several cases. For each case it applies a combination of marking followed by a filtering step, the Kangaroo method, or convolutions. The goal is to not exceed $O(n\sqrt{k\log k})$ time in any of the cases. We now present an algorithm with only two cases which has the same worst case run time. The new algorithm can be thought of as a generalization of the algorithm in [8] as we will discuss later. This generalization not only greatly simplifies the algorithm but it also reduces the expected run time. This happens because we use information about the frequency of the characters in the text and try to minimize the work done by convolutions and marking.

For any character $\alpha \in \Sigma$, let $f_{\alpha}$ be its frequency in the pattern, and $F_{\alpha}$ be its frequency in the text. Clearly, $\sum_{\alpha \in \Sigma} f_{\alpha} = m$ and $\sum_{\alpha \in \Sigma} F_{\alpha} = n$. A position $j$ in the pattern where $p[j] = \alpha$ is called an instance of $\alpha$. Consider every instance of character $\alpha$ as an object of size 1 and cost $F_{\alpha}$. We want to fill a knapsack of size $2k$ at a cost less than a given budget $B$. This problem can be optimally solved by a greedy approach where we include all the instances of the least expensive character, then all the instances of the second least expensive character and so on, until we have $2k$ items or we have exceeded $B$. The last character considered may have only a subset of its instances included, but for ease of explanation assume that there are no such characters.

The algorithm is the following: Case 1) If we can fill the knapsack within budget $B$, we apply the marking algorithm for the characters whose instances are included in the knapsack. If alignment $i$ matches perfectly, we will obtain exactly $2k$ marks at position $i$ in the text. Thus, any position which has less than $k$ marks must have more than $k$ mismatches. Based on this observation, we run Subset $k$-mismatches to check only those positions with at least $k$ marks.

Case 2) If we cannot fill the knapsack within the given budget we do the following: for the characters we could fit in the knapsack before we ran out of budget, we use the marking algorithm to count the number of matches they contribute to each alignment. For characters not in the knapsack, we use convolutions to count the number of matches they contribute to each alignment. We add the two counts and get the exact number of matches for every alignment. We call this algorithm Knapsack $k$-mismatches (also see algorithm 7 in the appendix).

Theorem 5: Knapsack $k$-mismatches has worst case run time $O(n\sqrt{k\log k})$.

Proof: In case 1, if we can fill the knapsack within budget $B$, we apply the marking algorithm. This takes $\sum_{\alpha \in \text{knapsack}} f_{\alpha} B = B$ time and creates just as many marks. Thus, there will be no more than $B/k$ positions with at least $k$ marks. We run Subset $k$-mismatches for these positions and obtain a run time of $O(n + m + B)$.

In case 2, if we cannot fill the knapsack within the given budget, we apply the marking algorithm for whatever items we could fit in the knapsack.
This takes $O(B)$ time. Note that if we add the costs of including in the knapsack all the instances of characters with frequency lower than $B/n$ we get $\sum_{f_a < B/n} f_a F_a < B/n \sum_{f_a} F_a = B$. We can include all of them in the knapsack by only adding a constant factor to the run time of the marking stage. Thus, we can assume that the characters not in the knapsack have frequency $f_a \geq B/n$. There cannot be more than $r = 2k/(B/n)$ characters not in the knapsack, otherwise we could have filled the knapsack within budget $B$ by picking $B/n$ instances for each of $r$ such characters, for a total of $2k$ positions and a cost $\sum_{i=1}^r B/n F_i \leq B$. Thus, it takes $O(rn \log m) = O(n^2 k \log m/B)$ time to compute convolutions for the characters not in the knapsack. If we make this cost equal to the cost of the marking phase, $O(B)$, we find $B = n \sqrt{k \log m}$. As in [8], if $k < m^{1/3}$ we can employ a different algorithm which solves the problem in linear time. For larger $k$, $O(\log m) = O(\log k)$ so the run time becomes $O(n \sqrt{k \log k})$.

We can think of the algorithm in [8] as a special case of our algorithm where, instead of trying to minimize the cost of the $2k$ items in the knapsack, we just try to find $2k$ of them for which the cost is less than $O(n \sqrt{k \log m})$. As a result, it is easy to verify the following:

**Theorem 6**: Knapsack $k$-mismatches spends at most as much time as the algorithm in [8] to do convolutions and marking.

**Proof**: In the appendix.

## 6 Experimental Results

It is interesting to analyze how some of the above algorithms compare in practice, since some of them are based on symbol comparison, some on arithmetic operations, and some on a combination of both. We implemented the following algorithms: the naive $O(nm)$ time algorithm, Abrahamson’s, Subset $k$-mismatches and Knapsack $k$-mismatches. For Subset $k$-mismatches, we simulate the suffix tree and LCA extensions by a suffix array with an LCP (Longest Common Prefix [17]) table and data structures to perform RMQ queries (Range Minimum Queries [18]) on it. This adds a $O(\log n)$ factor to preprocessing and searching. However, faster implementations are possible. For Subset $k$-mismatches, we also tried a simple $O(n^2)$ time pre-processing using dynamic programming and hashing. Knapsack $k$-mismatches uses Subset $k$-mismatches as a subroutine, so we have two versions of it also. We use all algorithms to solve the $k$-mismatches problem, even though some are more general.

We tested the algorithms on protein, DNA and English inputs from the Pizza & Chili Corpus [19]. These inputs were truncated at several thresholds, to analyze how run time varies with the length of the text. We randomly selected a substring of length $m$ from the text and used it as pattern. The algorithms were tested on an Intel Core i3 machine with 4GB of RAM, Ubuntu 11.10 Operating System and gcc 4.6.1. All convolutions were performed using the fftw library.

Figure 1 shows run times for varying $n, m, k$ and $[\Sigma]$. The naive algorithm performed well in practice most likely due to its simplicity and cache locality. Abrahamson’s algorithm, for alphabet sizes smaller than $\sqrt{m/\log m}$, computes one convolution for every character in the alphabet. The convolutions proved to be expensive in practice, so Abrahamson’s algorithm was competitive only for large $k$. Subset $k$-mismatches, applied for the full set of alignments, performed well for relatively small $k$. In most cases, the suffix array version was slower than the one with $O(n^2)$ time pre-processing, because of the added $O(\log n)$ factor when searching in the suffix array. Knapsack $k$-mismatches was the fastest among the algorithms compared because on most test instances the knapsack could be filled within the given budget. On such instances the algorithm did not perform convolution operations.

## 7 Conclusions

We have introduced several randomized and deterministic, exact and approximate algorithms for pattern matching with mismatches and the $k$-mismatches problems, with or without wild cards. These algorithms improve the run time, simplify, or extend previous algorithms to accommodate wild cards. We implemented the deterministic algorithms. An empirical comparison of these algorithms showed that those based on character comparison outperformed those based on convolutions.

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Fig. 1. Run times for the tested algorithms. M stands for millions. Top row: k varies. Second row: m varies. Third row: n varies. Bottom row: alphabet size varies, legend.

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APPENDIX A

ALGORITHM 6 - SUBSET k-MISMATCHES

Algorithm 6 Subset k-mismatches(S)
  // S = set of positions to test
  let M_i := 0 for all i ∈ 1, n
  i := 1
  while i ≤ n do
    find the largest l such that ∃j for which
    T_{i..i+l−1} = P_{j..j+l−1}
    for all s ∈ S where s ≤ i < s + m do
      M_s := updateMism(M_s, i − s + 1, j, l)
    end for
    if M_s > k then
      S := S − {s}
    end if
    i := i + 1
  end while
  return M

function updateMism(c, s1, s2, l)
  while l > 0 and c ≤ k do
    d := lca(s1, s2)
    if d ≥ l then return c
    c := c + 1
    d := d + 1
    s1 := s1 + d
    s2 := s2 + d
    l := l − d
  end while
  return c

APPENDIX B

ALGORITHM 7 - KNAPSACK k-MISMATCHES

Algorithm 7 Knapsack k-mismatches
  compute F_i and f_i for every i ∈ Σ
  sort Σ with respect to F_i
  s := 0
  c := 0
  i := 1
  B := n√k log k
  while s < 2k and c < B do
    t := min(f_i, 2k − s)
    s := s + t
    c := c + t * F_i
  end while

APPENDIX C

PROOF OF THEOREM 6

Theorem 6 states that Knapsack k-mismatches will spend at most as much time as the algorithm in [8] to do convolutions and marking.

Proof: Observation: In all the cases presented below, Knapsack k-mismatches can have a run time as low as O(n), for example if there exists one character α with f_α = O(k) and F_α = O(n/k).

Case 1: |Σ| ≥ 2k. The algorithm in [8] chooses 2k instances of distinct characters to perform marking. This ensures that the cost M of the marking phase is less or equal to n and the number of remaining positions after filtering is no more than M/k. Our algorithm puts in the knapsack 2k instances of not necessarily different characters such that the cost B of the marking phase is minimized. Clearly B ≤ M and the number of remaining positions after filtering is less or equal to B/k ≤ M/k.

Case 2: |Σ| < 2√k. The algorithm in [8] performs one convolution per character to count the total number of matches for every alignment, for a run time of O(|Σ|n log m). Only in the worst case, Knapsack k-mismatches cannot fill the knapsack at a cost B < |Σ|n log m so it defaults to the same run time. However, in the best case, the knapsack can be filled at a cost B as low as O(n) and so the run time could be linear.

Case 3: 2√k ≤ |Σ| ≤ 2k. A symbol that appears in the pattern at least 2√k times is called frequent.

Case 3.1: There are at least √k frequent symbols. The algorithm in [8] chooses 2√k instances of √k frequent symbols to do marking and filtering at a cost M ≤ 2n√k. Since Knapsack k-mismatches will minimize the time B of the marking phase we have B ≤ M so in the worst case the run time is the same as for [8].

Case 3.2: There are A < √k frequent symbols. The algorithm in [8] first performs one convolution for
each frequent character for a run time of \( O(An \log m) \).

Two cases remain:

**Case 3.2.1:** All the instances of the non-frequent symbols number less than \( 2k \) positions. The algorithm in [8] replaces all instances of frequent characters with wild cards and applies a \( O(n \sqrt{g} \log m) \) algorithm to count mismatches, where \( g \) is the number of non-wild card positions. Since \( g < 2k \) the run time for this stage is \( O(n \sqrt{k} \log m) \) and the total run time is \( O(An \log m + n \sqrt{k} \log m) \). Knapsack \( k \)-mismatches can always include in the knapsack all the instances of non-frequent symbols since their total cost is no more than \( O(n \sqrt{k}) \) and in the worst case do convolutions for the remaining characters at a total run time of \( O(An \log m + n \sqrt{k}) \). In practice, the knapsack will be filled using some instances of both frequent and infrequent characters, whichever minimize the cost.

**Case 3.2.2:** All the instances of the non-frequent symbols number at least \( 2k \) positions. The algorithm in [8] chooses \( 2k \) instances of infrequent characters to do marking. Since each character has frequency less than \( 2\sqrt{k} \), the time for marking is \( M < 2n \sqrt{k} \) and there are no more than \( M/k \) positions left after filtering. Knapsack \( k \)-mismatches chooses characters in order to minimize the time \( B \) for marking, so \( B \leq M \) and there are no more than \( B/k \leq M/k \) positions left after filtering.