Approximate String Matching Giulia Bernardini giulia.bernardini@units.it

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From exact to approximate string matching

- Often in applications we want to search a text for something that is similar to the pattern but not necessarily exactly the same.
- This is the case, for example, when we want to search for a word in a text taking possible typos into account; or when we want to map a read in a genome taking into account sequencing errors.
- To formalize this problem, we have to specify what does "similar" mean. This can be done by defining a distance measure for strings.

From exact to approximate string matching

There are several possible ways to define distances between strings. Let us start with the simplest notion, which is a measure of distance between two strings of the same length.

Given two strings S and T, both of length n, the Hamming distance between S and T is the number of positions i such that $S[i] \neq T[i]$. The following two strings have Hamming distance 3.

TATGTTACAA AATCTTACAC

Computing the Hamming distance between S and T requires (trivially) O(n) time.

The Hamming distance

Hamming distance is a metric on Σ^n , for any fixed alphabet Σ and string length n. Let us denote by $d_H(S,T)$ the Hamming distance between strings S and T, both in Σ^n .

- $d_H(S,T) \ge 0$ for any S,T
- $d_H(S,T)=d_H(T,S)$
- $d_H(S,T)=0$ if and only if S=T
- d_H(S,T)≤d_H(S,U)+d_H(U,T). Indeed, for positions i s.t. S[i]≠T[i], it must be either S[i]≠U[i] or U[i]≠T[i] (or both).

S=TATGTTACAA IIIXIIIXII U=TATCTTAGAA XIIIIXIX T=AATCTTACAC

 $d_H(S,T)=3; d_H(S,U)=2; d_H(U,T)=3$

The k-mismatch problem

Reference: Chapters 9.1 and 9.4 of: Gusfield, D. *Algorithms on Strings, Trees and Sequences.*

The k-mismatch problem

IN: a text T of length n, a pattern P of length m<n, an integer k<m **OUT:** all positions i in T such that $d_H(T[i..i+|P|-1],P) \le k$

```
7 10 13 16
T=AMBARABACCICCICCOCCO ; P=COCCO ; k=3
COCCO
COCCO
COCCO
COCCO
COCCO
```

```
Output: {7,10,13,16}
```

The k-mismatch problem

Theorem. Given a text T of length n, a pattern P of length m < n, and an integer k < m, the k-mismatch problem can be solved in O(kn) time, after an O(n+m)-time preprocessing.

Longest Common Extension queries

Problem: preprocess two strings S and T such that the following queries can be answered efficiently.

Query: given a position i in S and a position j in T, find the length of the longest common prefix (called Longest Common Extension) of S[i..|S|] and T[j..|T|], denoted by $LCE_{S,T}(i,j)$.

Example. Let S=abracadabra, T=bracco. Then: $LCE_{S,T}(2,1)=4$ abracadabra
bracco $LCE_{S,T}(6,3)=1$ abradadabra
bracco $LCE_{S,T}(7,4)=0$ abracadabra
bracco

Longest Common Extension queries

Theorem. Given a string S of length n and a string T of length m, LCE queries can be answered in O(1) time after an O(n+m)-time preprocessing.

The preprocessing required is to build the generalised suffix tree of S and T, and then to preprocess it to allow constant-time LCA queries.

Then $LCE_{S,T}(i,j)$ is equal to the string depth of $LCA(u_i,v_j)$, where u_i is the leaf of the generalised suffix tree corresponding to S[i..|S|], v_j is the leaf of the generalised suffix tree corresponding to T[j..|T|].

Lowest Common Ancestor queries

- The lowest common ancestor (LCA) of two nodes u and v is the deepest node that is an ancestor of both u and v.
- **Theorem (Bender and Farach-Colton).** Any tree of size O(N) can be preprocessed in O(N) time so that the LCA of any two nodes can be computed in O(1) time.



The kangaroo algorithm for k-mismatch

```
kMISMATCH(T,P,k)
   sol \leftarrow \emptyset;
   for all i=1,...,|T|
      count \leftarrow 0; match \leftarrow 0;
      while count <k and match+count <|P|
          ext←LCE<sub>T,P</sub>( match+count+i , match+count+1 );
          match \leftarrow match + ext;
         if match+count=|P|
             sol.append(i);
         else
            count \leftarrow count +1;
   return sol;
```



The edit distance problem

Reference: Chapters 11.2 and 11.3 of: Gusfield, D. Algorithms on Strings, Trees and Sequences.

The edit distance between two strings

The most widely used notion of distance between strings is a measure of distance between two strings of any lengths that focuses on transforming one string into the other with a series of edit operations on individual characters.

The permitted operations are deleting a character from the first string, (denoted by D) inserting a character in the first string (I), or replacing a character of the first string with another (R).

Given two strings S and T, both of length n, the edit distance between S and T is the minimum number of character deletions, insertions and replacements to transform S into T.

The following two strings have edit distance 5. S=VINT NER T= INTEREST D IR RI

The edit distance between two strings

Note that there may be multiple sequences of edit operations of minimum length that transform S into T: the edit distance is just the minimum length.

```
S=VINT NER
T= INTEREST
D IR RI
```

S=VINT NE R T= INTEREST D IR IR

```
S=VINTNER
T= INT EREST
D D III
```

The edit distance between two strings

Note that there may be multiple sequences of edit operations of minimum length that transform S into T: the edit distance is just the minimum length.

S=VINT NER DMMMIRMRI

S=VINT NE R T = INTEREST T = INTERESTDMMMIRMIR

S=VINTNER T = INT ERESTDMMMDMMIII

Using "M" to denote a non-operation "match" in addition to the symbols of the three edit operations "I", "D", "R", a string over the alphabet {M,I,D,R} that describes a transformation of S into T is called an edit transcript of the two strings.

The edit distance problem

Given two strings S and T, the edit distance problem is to compute the edit distance between S and T together with an optimal edit transcript that describes a minimum-length transformation.

Theorem. The edit distance between a string S and a string T can be computed in O(|S||T|) time and space.

This problem can be solved with a dynamic programming algorithm.

Given strings S of length n and T of length m, we denote by D(i,j) the edit distance between S[1..i] and T[1..j]. D(n,m) denotes the edit distance between the whole S and T.

Base conditions: D(i,0)=i (i deletions) and D(0,j)=j (j insertions).

Let d:[1,n]x[1,m] \rightarrow {0,1} a function such that d(i,j)=1 if S[i] \neq S[j], d(i,j)=0 otherwise. Then it holds the following

Recursion: $D(i,j)=min\{ D(i-1,j)+1 , D(i,j-1)+1 , D(i-1,j-1)+d(i,j) \}$ for any $i \in [1,n], j \in [1,m]$.

Lemma 1. For any $i \in [1,n]$, $j \in [1,m]$, D(i,j) is either D(i-1,j)+1, D(i,j-1)+1, or D(i-1,j-1)+d(i,j). There are no other possibilities.

Proof. Consider an optimal transcript for S[1..i] and T[1..j], and focus on the last operation. There are four cases.

1. The last operation is the insertion of T[j] at the end of the transformed S[1..i]. Then the transcript before the last symbol I gives the minimum number of operations to transform S[1..i] into T[1..j-1], and this number is precisely D(i,j-1). Adding 1 for the last insertion, we obtain that D(i,j)=D(i,j-1)+1.

S=VINT T= INTE DMMMI i=4,j=4, D(4,4)=2, D(4,3)=1

Lemma 1. For any $i \in [1,n]$, $j \in [1,m]$, D(i,j) is either D(i-1,j)+1, D(i,j-1)+1, or D(i-1,j-1)+d(i,j). There are no other possibilities.

Proof. Consider an optimal transcript for S[1..i] and T[1..j], and focus on the last operation. There are four cases.

2. The last operation is the deletion of S[i]. Then the transcript before the last symbol D gives the minimum number of operations to transform S[1..i-1] into T[1..j], and this number is precisely D(i-1,j). Adding 1 for the last deletion, we obtain that D(i,j)=D(i-1,j)+1.

S=VINTN T= INT DMMMD i=5,j=3, D(5,3)=2, D(4,3)=1

Lemma 1. For any $i \in [1,n]$, $j \in [1,m]$, D(i,j) is either D(i-1,j)+1, D(i,j-1)+1, or D(i-1,j-1)+d(i,j). There are no other possibilities.

Proof. Consider an optimal transcript for S[1..i] and T[1..j], and focus on the last operation. There are four cases.

3. The last operation is the replacement of S[i] with T[j]. Then the transcript before the last symbol R gives the minimum number of operations to transform S[1..i-1] into T[1..j-1], and this number is precisely D(i-1,j-1). Adding 1 for the last replacement, we obtain that D(i,j)=D(i-1,j-1)+1.

```
S=VINT N
T= INTER
DMMMIR
i=5,j=5, D(5,5)=3, D(4,4)=2
```

Lemma 1. For any $i \in [1,n]$, $j \in [1,m]$, D(i,j) is either D(i-1,j)+1, D(i,j-1)+1, or D(i-1,j-1)+d(i,j). There are no other possibilities.

Proof. Consider an optimal transcript for S[1..i] and T[1..j], and focus on the last operation. There are four cases.

4. Finally, if the last symbol is the match S[i]=T[j]. Then D(i,j)=D(i-1,j-1).

S=VINT T= INT DMMM i=4,j=3, D(4,3)=1, D(3,2)=1

Lemma 2. For any $i \in [1,n]$, $j \in [1,m]$, $D(i,j) \le \min\{D(i-1,j)+1, D(i,j-1)+1, D(i-1,j-1)+d(i,j)\}$

Proof. With the same reasoning of the proof of Lemma 1, it suffices to show that for each case there exists a transformation achieving each of the three values specified in the lemma statement.

The dynamic programming algorithm for computing edit distance consists in computing all values D(i,j) bottom-up, starting from the smallest possible i and j and storing the computed values in a dynamic programming table that has the letters of S at the columns and the letters of T at the rows (plus an extra row and column to account for i=0 and j=0).

Column and row 0 are filled in using the base conditions.

		S	u	n	d	а	У
	0	1	2	3	4	5	6
S	1						
а	2						
t	3						
u	4						
r	5						
d	6						
а	7						
У	8						

Column and row 0 are filled in using the base conditions. The other cells are filled in using the recursive relation.

		S	u	n	d	а	У
	0	1	2	3	4	5	6
S	1	0	1				
а	2	1					
t	3						
u	4						
r	5						
d	6						
а	7						
у	8						

Column and row 0 are filled in using the base conditions. The other cells are filled in using the recursive relation. The result is in the bottom-right cell.

		S	u	n	d	а	У
	0	1	2	3	4	5	6
S	1	0	1	2	3	4	5
а	2	1	1	2	3	3	4
t	3	2	2	2	3	4	4
u	4	3	2	3	3	4	5
r	5	4	3	3	4	4	5
d	6	5	4	4	3	4	5
а	7	6	5	5	4	3	4
У	8	7	6	6	5	4	3

Computing edit distance: traceback

In order to reconstruct an optimal transcript, it suffices to store some pointers when computing the table: when computing D(i,j) we store a pointer from cell (i,j) to cell (i-1,j) if D(i,j)=D(i-1,j)+1; we store a pointer to cell (i,j-1) if D(i,j)=D(i,j-1)+1; we store a pointer to cell (i-1,j-1) if D(i,j)=D(i-1,j-1)+d(i,j).

We can then follow any pointer path from cell (m,n) to cell (0,0). This way we reconstruct a transcript backwards, writing an I every time we follow a vertical pointer, a D every time we follow a horizontal pointer, and a R or a M when we follow a diagonal pointer, depending on the value of function d.

The optimal transcript highlighted in grey is MIIMRMMM, corresponding to the alignment

S unday Saturday MIIMRMMM

		S	u	n	d	а	У
	0	1	2	3	4	5	6
S	1	0	1	2	3	4	5
а	2	1	1	2	3	3	4
t	3	2	2	2	3	4	4
u	4	3	2	3	3	4	5
r	5	4	3	3	4	4	5
d	6	5	4	4	3	4	5
а	7	6	5	5	4	3	4
У	8	7	6	6	5	4	3