Approximating Longest Common Substring with k mismatches

Garance Gourdel, Tomasz Kociumaka, Jakub Radoszewski, Tatiana Starikovskaya

Similarity measures

Given two strings *X* and *Y*, how similar are they?

Ideally, we want a similarity measure that is

- ► Robust: Small change in the input ⇒ small change of the measure
- ► Fast to compute

Applications in Bioinformatics, Information Retrieval.

Edit distance

Smallest number of **insertions**, **deletions**, and **substitutions** required to convert one string into the other.

EditDistance(GATTACAT, ATTACATT) = 2

Can be computed in quadratic time using dynamic programming. This is probably optimal:

[Backurs and Indyk'15] The Edit distance can't be computed in strongly subquadratic time, unless SETH is false.

SETH (Strong Exponential Time Hypothesis)

 $\forall \delta > 0$, there exists an integer q such that SAT on q-CNF formulas with m clauses and n variables cannot be solved in time $m^{O(1)}2^{(1-\delta)n}$.

Longest Common Substring

The maximal length of a string that occurs in both strings.

$$LCS (TAAGC, AAGAA) = 3$$

Can be computed in $\mathcal{O}(n)$ time [Hui'92].

Unfortunately, not robust: can change a lot when we change a few characters of the input.

This work

Longest Common Substring with *k* mismatches problem

Input: an integer k, strings S_1 , S_2 of length n

Output: the maximal length of a substring of S_1 that occurs in S_2 with k mismatches

$$LCS_k$$
 (TAAGC, AAGAA) = 4 for $k = 1$

Closely related to the *k*-macs (the *k*-mismatch average common substring) distance [Leimeister, Morgenstern'14]

Longest Common Substring with *k* mismatches

Exact solutions:

- ▶ k = 1: $\mathcal{O}(n \log n)$ time [Flouri et al.'15]
- ▶ $\mathcal{O}(n^2)$ time dyn. prog. [Flouri et al.'15]
- ► $\mathcal{O}(n((k+1)(|\mathsf{LCS}|+1))^k)$ or $\mathcal{O}(n^2|\mathsf{LCS}_k|/k)$ time [Grabowski'15]
- $ightharpoonup k^{1.5} n^2/2^{\Omega(\sqrt{\frac{\log n}{k}})}$ time, rand. [Abboud et al.'15]
- $\triangleright \mathcal{O}(n \log^k n)$ time [Thankachan et al.'16]
- ► $LCS_k \ge \log^{2k+2} n$: O(n) time [Charalampopoulos et al.'18]

All solutions use $\mathcal{O}(n)$ space.

In general, LCS $_k$ cannot be solved in strongly subquadratic time, unless SETH is false [Kociumaka et al.'19]

Longest Common Substring with approx. *k* mismatches

Input: an integer k, a constant $\varepsilon > 0$, strings S_1, S_2 of length n

Output: The length $LCS_{\tilde{k}} \ge LCS_k(T_1, T_2)$ of a substring of S_1 that occurs in S_2 with $\le (1 + \varepsilon) \cdot k$ mismatches

$$S_1 = TAAGCTTT$$
, $S_2 = CACGTTTC$, $k = 2$, $\varepsilon = 1.5$
 $LCS_k(S_1, S_2) = 6 \Rightarrow$ we can return AGCTTT

- ▶ More robust than LCS, easier to compute
- ▶ $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log^2 n)$ time, $\mathcal{O}(n^{1+1/(1+\varepsilon)})$ space for any $0 < \varepsilon < 2$ [Kociumaka et al.'19]
- ► Main idea: locality-sensitive hashing
- ▶ Very complex system of hash functions, superlinear space

Longest Common Substring with approx. *k* mismatches

Input: an integer k, a constant $\varepsilon > 0$, strings S_1, S_2 of length n

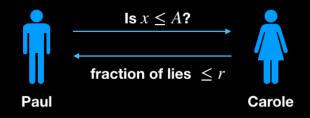
Output: The length $LCS_{\tilde{k}} \ge LCS_k(T_1, T_2)$ of a substring of S_1 that occurs in S_2 with $\le (1 + \varepsilon) \cdot k$ mismatches

$$S_1 = TAAGCTTT$$
, $S_2 = CACGTTTC$, $k = 2$, $\varepsilon = 1.5$
 $LCS_k(S_1, S_2) = 6 \Rightarrow$ we can return AGCTTT

- ▶ More robust than LCS, easier to compute
- $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log^3 n)$ time, $\mathcal{O}(n)$ space for any $\varepsilon > 0$ [This work]
- ► Main idea: locality-sensitive hashing
- ▶ Practical: Simple system of hash functions, linear space

Reduction to the decision variant

Twenty question game with a liar



Given $0 \le A, B \le n$. Carole must answer YES if $x \le A$ and NO if x > B. To win, Paul must return some number in [A, B].

Corollary of [Dhagat, Gács, Winkler '92]: For any $r<\frac{1}{3}$, Paul can win by asking $\lceil \frac{8\log n}{(1-3r)^2} \rceil$ questions.

Decision variant

Input: integers k, ℓ , a constant $\varepsilon > 0$, strings S_1, S_2 of length n Output:

- 1. YES if $\ell \leq LCS_k$;
- 2. YES or NO if $LCS_k < \ell \le LCS_{(1+\varepsilon)k}$;
- 3. NO if LCS_{$(1+\varepsilon)k$} $< \ell$.

The answer must be correct with probability at least 3/4.

Longest Common Substring with approx. *k* mismatches:

- ▶ $A = LCS_k$ and $B = LCS_{(1+\varepsilon)k}$.
- An algorithm for the decision variant plays the role of Carole.
- ▶ With $\lceil \frac{8 \log n}{(1-3r)^2} \rceil$ questions, Paul will find $x \in [LCS_k, LCS_{(1+\varepsilon)k}]$ for some 1/4 < r < 1/3.

Decision variant

Input: integers k, ℓ , a constant $\varepsilon > 0$, strings S_1, S_2 of length n Output:

- 1. YES if $\ell \leq LCS_k$;
- 2. YES or NO if LCS_k $< \ell \le LCS_{(1+\varepsilon)k}$;
- 3. NO if LCS_{$(1+\varepsilon)k$} $< \ell$.

The answer must be correct with probability at least 3/4.

Longest Common Substring with approx. k mismatches:

- ► $A = LCS_k$ and $B = LCS_{(1+\varepsilon)k}$.
- ► An algorithm for the decision variant plays the role of Carole.
- ▶ With $\lceil \frac{8 \log n}{(1-3r)^2} \rceil$ questions, Paul will find $x \in [LCS_k, LCS_{(1+\varepsilon)k}]$ for some 1/4 < r < 1/3.

Definition: A family \mathcal{F} of hash functions is called *locality-sensitive*, if for all $X, Y \in \Sigma^n$ and a hash function $h \in \mathcal{F}$ chosen u.a.r.:

- ▶ If $\operatorname{Ham}(X, Y) \leq k$, then h(X) = h(Y) with prob. $\geq p_1$;
- ▶ If $\operatorname{Ham}(X,Y) \geq (1+\varepsilon)k$, then h(X) = h(Y) with prob. $\leq p_2$.

Main idea (simplified):

We choose a locality-sensitive hash function $h \in \mathcal{F}$ uniformly at random, and apply it to all ℓ -length substrings of S_1, S_2 .

We then explore the pairs of strings that collide

If there is a pair of ℓ -length substrings of X,Y with k mismatches, we will find it.

Definition: A family \mathcal{F} of hash functions is called *locality-sensitive*, if for all $X, Y \in \Sigma^n$ and a hash function $h \in \mathcal{F}$ chosen u.a.r.:

- ▶ If $\operatorname{Ham}(X, Y) \leq k$, then h(X) = h(Y) with prob. $\geq p_1$;
- ▶ If $\operatorname{Ham}(X,Y) \geq (1+\varepsilon)k$, then h(X) = h(Y) with prob. $\leq p_2$.

Main idea (simplified):

We choose a locality-sensitive hash function $h \in \mathcal{F}$ uniformly at random, and apply it to all ℓ -length substrings of S_1, S_2 .

We then explore the pairs of strings that *collide*.

If there is a pair of ℓ -length substrings of X,Y with k mismatches, we will find it.

We construct hash functions as in [Indyk and Motwani'98]:

$$\Pi = \{h_i, 1 \le i \le n : h_i(a_1 a_2 \dots a_n) = a_i\}$$

 $\mathcal{F} = \Pi^m$ for some parameter m

How to compute the collisions for $h \in \mathcal{F}$? We use Karp–Rabin fingerprints: $h(X) \neq h(Y) \Rightarrow \varphi(h(X)) \neq \varphi(h(Y)) \Rightarrow w / \text{prob. } 1 - 1/n$

The fingerprints can be computed in $O(n \log n)$ time via FFT

Choice of parameters:

$$\begin{aligned} p_1 &= 1 - k/n, p_2 = 1 - (1+\varepsilon) \cdot k/n \\ m &= \log_{p_2} \lceil 1/n \rceil \end{aligned}$$

We construct hash functions as in [Indyk and Motwani'98]:

$$\Pi = \{h_i, 1 \le i \le n : h_i(a_1 a_2 \dots a_n) = a_i\}$$

 $\mathcal{F} = \Pi^m$ for some parameter m

How to compute the collisions for $h \in \mathcal{F}$? We use Karp–Rabin fingerprints: $h(X) \neq h(Y) \Rightarrow \varphi(h(X)) \neq \varphi(h(Y)) \Rightarrow w / \text{prob. } 1 - 1/n^c$

The fingerprints can be computed in $O(n \log n)$ time via FFT

Choice of parameters

$$\begin{aligned} p_1 &= 1 - k/n, p_2 = 1 - (1 + \varepsilon) \cdot k/n \\ m &= \log_{p_2} \lceil 1/n \rceil \end{aligned}$$

We construct hash functions as in [Indyk and Motwani'98]:

$$\Pi = \{h_i, 1 \le i \le n : h_i(a_1 a_2 \dots a_n) = a_i\}$$

 $\mathcal{F} = \Pi^m$ for some parameter m

How to compute the collisions for $h \in \mathcal{F}$? We use Karp–Rabin fingerprints: $h(X) \neq h(Y) \Rightarrow \varphi(h(X)) \neq \varphi(h(Y)) \Rightarrow w / \text{prob. } 1 - 1/n^c$

The fingerprints can be computed in $O(n \log n)$ time via FFT

Choice of parameters:

$$\begin{aligned} p_1 &= 1 - k/n, p_2 = 1 - (1 + \varepsilon) \cdot k/n \\ m &= \log_{p_2} \lceil 1/n \rceil \end{aligned}$$

Algorithm

- 1: Choose a set $\mathcal H$ of $\Theta(n^{1/(1+\varepsilon)})$ functions from Π^m u.a.r.
- 2: $C_l^{\mathcal{H}}:=$ set of all collisions of l-length substrings of S_1,S_2 under the hash functions in \mathcal{H}
- 3: Draw a collision $(X, Y) \in C_{\ell}^{\mathcal{H}}$ uniformly at random
- 4: **if** $Ham(X, Y) \le (1 + \varepsilon) \cdot k$ then return YES
- 5: Choose a subset $C' \subseteq C_l^{\mathcal{H}}$ of size $\min\{C_\ell^{\mathcal{H}}, 4nL\}$
- 6: for $(X, Y) \in C'$ do
- 7: **if** $Ham(S_1, S_2) \le k$ then return YES
- 8: return NO

Running time $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log n)$:

- 1. Compute the hash values and C': $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log n)$ time (FFT)
- 2. Pick a random collision: $\mathcal{O}(n^{1+1/(1+\varepsilon)})$ time (reservoir sampling)
- 3. Test in line 5: $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log^2 n)$ time (dimension reduction)
- 4. Test in line 7: $\mathcal{O}(n)$ time (character-by-character

Algorithm

- 1: Choose a set \mathcal{H} of $\Theta(n^{1/(1+\varepsilon)})$ functions from Π^m u.a.r.
- 2: $C_l^{\mathcal{H}}:=$ set of all collisions of l-length substrings of S_1,S_2 under the hash functions in \mathcal{H}
- 3: Draw a collision $(X,Y) \in C^{\mathcal{H}}_{\ell}$ uniformly at random
- 4: **if** $Ham(X, Y) \le (1 + \varepsilon) \cdot k$ **then return** YES
- 5: Choose a subset $C' \subseteq C_l^{\mathcal{H}}$ of size $\min\{C_\ell^{\mathcal{H}}, 4nL\}$
- 6: for $(X, Y) \in C'$ do
- 7: **if** $Ham(S_1, S_2) \le k$ then return YES
- 8: return NO

Running time $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log n)$:

- 1. Compute the hash values and C': $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log n)$ time (FFT)
- 2. Pick a random collision: $\mathcal{O}(n^{1+1/(1+\varepsilon)})$ time (reservoir sampling)
- 3. Test in line 5: $\mathcal{O}(n^{1+1/(1+\varepsilon)}\log^2 n)$ time (dimension reduction)
- 4. Test in line 7: $\mathcal{O}(n)$ time (character-by-character)

Experiments

None of the previous solutions have been implemented.

The only algorithm that seemed to be practical enough is the dynamic programming one [Flouri et al.'15]

We compared our algorithm with the dynamic programming one

- ► On random strings;
- ▶ On strings extracted from E. coli.

Lengths from 5000 to 60000, k = 10, 25, 50

Experiments

None of the previous solutions have been implemented.

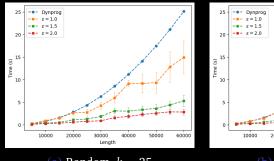
The only algorithm that seemed to be practical enough is the dynamic programming one [Flouri et al.'15]

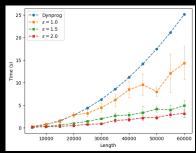
We compared our algorithm with the dynamic programming one

- ► On random strings;
- ▶ On strings extracted from E. coli.

Lengths from 5000 to 60000, k = 10, 25, 50

Running time





(a) Random, k = 25

- (b) E. coli, k = 25
- ► For each length, we performed 10 independent experiments
- ▶ Big standard deviation for $\varepsilon = 1$, negligible for $\varepsilon = 1.5$ and $\varepsilon = 2.0$
- ► Gain up to a factor of 10 on strings of length 60000

Distortion and accuracy

We estimate distortion by computing two values:

$$\begin{aligned} r_{\min}(\varepsilon, k) &= \min_{S_1, S_2}(\text{LCS}_{\tilde{k}}(S_1, S_2) / \text{LCS}_k(S_1, S_2)) \\ r_{\max}(\varepsilon, k) &= \max_{S_1, S_2}(\text{LCS}_{\tilde{k}}(S_1, S_2) / \text{LCS}_k(S_1, S_2)) \end{aligned}$$

Furthermore, we can only err by returning a string shorter than LCS_k .

	Random		
	arepsilon=1.0	arepsilon=1.5	arepsilon=2.0
k = 10	0.92 1.50	1.00 1.53	1.13 1.87
	err = 7%	err = 0%	err = 0%
k = 25	1.10 1.48	1.30 1.70	1.55 2.11
	err = 0%	err = 0%	err = 0%
		E. coli	
	arepsilon=1.0	E. coli $\varepsilon = 1.5$	arepsilon=2.0
k – 10	$arepsilon=1.0 \ 0.86 \ \ 1.41$		$arepsilon=2.0$ 0.95 $\mid 1.71$
k = 10		$\varepsilon=1.5$	
k = 10 $k = 25$	0.86 1.41	$\varepsilon = 1.5$ 0.91 1.47	0.95 1.71

Conclusion

- ► Longest common substring with *k* mismatches cannot be solved in subquadratic time unless SETH is false
- ▶ New approximation algorithm solves the problem in $\mathcal{O}(\mathbf{n}^{1+1/(1+\varepsilon)}\log^3\mathbf{n})$ time and $\mathcal{O}(\mathbf{n})$ space
- ▶ Simple and practical faster than the dynamic programming solution for $\varepsilon > 1$
- ► Small distortion compared to LCS_k (even though no theoretical guarantee)
- ▶ Good accuracy

Thank you!