

TARTU ÜLIKOO
ARVUTITEADUSE INSTITUUT

Text Algorithms (6EAP)

Full text indexing

Jaak Vilo
2010 fall

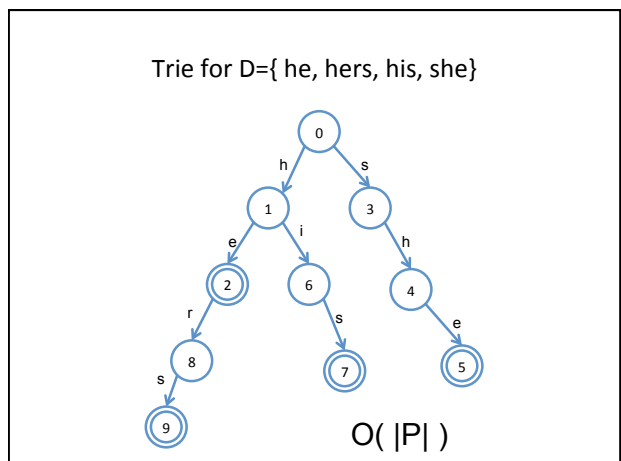
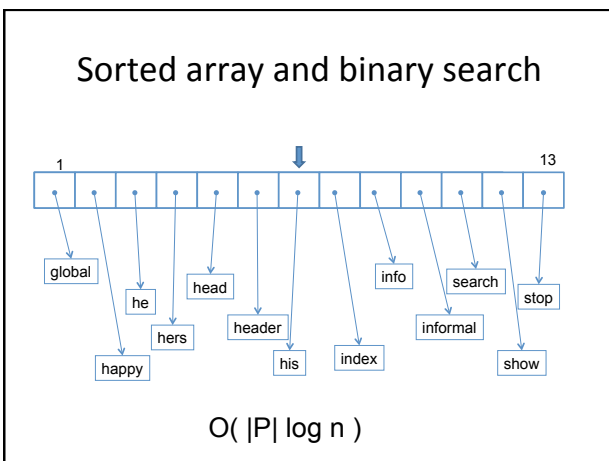
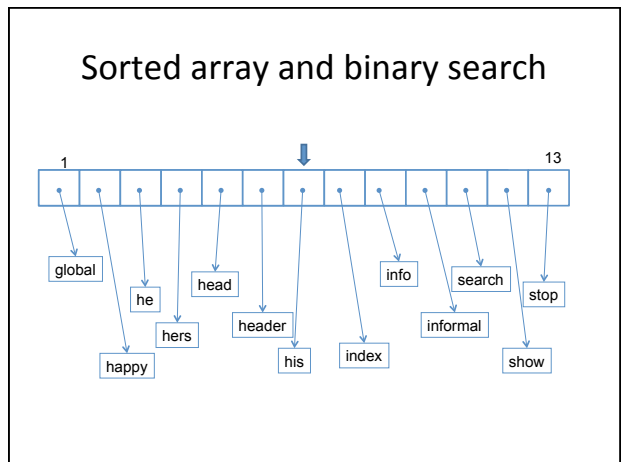
Jaak Vilo MTAT.03.190 Text Algorithms 1

Problem

- Given P and S – find all exact or approximate occurrences of P in S
- You are allowed to preprocess S (and P, of course)
- Goal: to speed up the searches

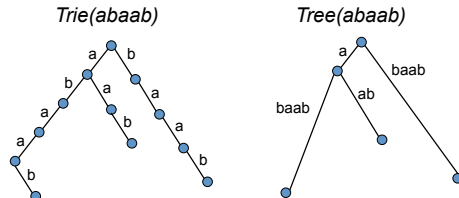
E.g. Dictionary problem

- Does P belong to a dictionary $D=\{d_1, \dots, d_n\}$
 - Build a binary search tree of D
 - B-Tree of D
 - Hashing
 - Sorting + Binary search
- Build a keyword trie: search in $O(|P|)$
 - Assuming alphabet has up to a constant size c
 - See Aho-Corasick algorithm, Trie construction



Suffix trie and suffix tree

abaab
baab
aab
ab
b



E. Ukkonen: <http://www.cs.helsinki.fi/u/ukkonen/Erice2005.ppt>

Suffix tree and suffix array techniques for pattern analysis in strings

Esko Ukkonen

Univ Helsinki

Erice School 30 Oct 2005

E. Ukkonen: <http://www.cs.helsinki.fi/u/ukkonen/Erice2005.ppt>

Algorithms for combinatorial string matching?

- deep beauty? +-
- shallow beauty? +
- applications? ++
- intensive algorithmic miniatures
- sources of new problems:
text processing, DNA, music,...

E. Ukkonen: <http://www.cs.helsinki.fi/u/ukkonen/Erice2005.ppt>

High-throughput genome-scale sequence analysis and mapping using compressed data structures

Veli Mäkinen

Department of Computer Science

University of Helsinki

tttttttttttgagacggagtctcgctctg
tcgccaggctggagtgcagtgccggg
atctcggctcactgcaagctccgcctcc
cgggttcagccattctcctcagcc
tccaagtagctgggactacaggcgc
cgccactacgccggctaattttgtattt
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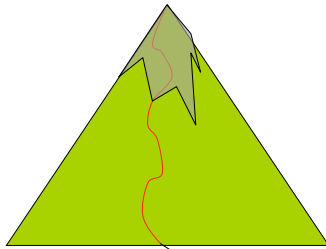
E. Ukkonen: <http://www.cs.helsinki.fi/u/ukkonen/Erice2005.ppt>

Analysis of a string of symbols

- T = hattivatti 'text'
- P = att 'pattern'
- Find the occurrences of P in T:
h a t t i v a t t i
- Pattern synthesis: #(*t*) = 4 #(*atti*) = 2 #(*t****t*) = 2

E. Ukkonen: <http://www.cs.helsinki.fi/u/ukkonen/Erice2005.ppt>

Solution: backtracking with suffix tree



...ACACATTATCACAGGCATCGGCATTAGCGATCGAGTCG.....

ISMB 2009 Tutorial

Veli Mäkinen: "...analysis and mapping..."

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Pattern finding & synthesis problems

- $T = t_1 t_2 \dots t_n, P = p_1 p_2 \dots p_n$, strings of symbols in finite alphabet
- **Indexing problem:** Preprocess T (build an index structure) such that the occurrences of different patterns P can be found fast
 - static text, any given pattern P
- **Pattern synthesis problem:** Learn from T new patterns that occur surprisingly often
- **What is a pattern?** Exact substring, approximate substring, with generalized symbols, with gaps, ...

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1. **Suffix tree**
2. Suffix array
3. Some applications
4. Finding motifs

E. Ukkonen: <http://www.cs.helsinki.fi/u/ukkonen/Erice2005.ppt>

The suffix tree $Tree(T)$ of T

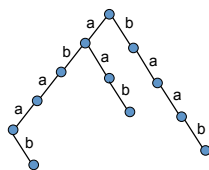
- data structure **suffix tree**, $Tree(T)$, is compacted trie that represents all the suffixes of string T
- linear size: $|Tree(T)| = O(|T|)$
- can be constructed in linear time $O(|T|)$
- has *myriad virtues* (A. Apostolico)
- is well-known: 366 000 Google hits

E. Ukkonen: <http://www.cs.helsinki.fi/u/ukkonen/Erice2005.ppt>

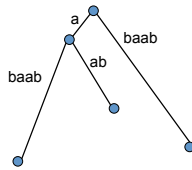
Suffix trie and suffix tree

abaab
baab
aab
ab
b

Trie(abaab)



Tree(abaab)



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Trie(T) can be large

- $|Trie(T)| = O(|T|^2)$
- bad example: $T = a^n b^n$
- Trie(T) can be seen as a DFA: language accepted = the suffixes of T
- minimize the DFA => directed cyclic word graph ('DAWG')

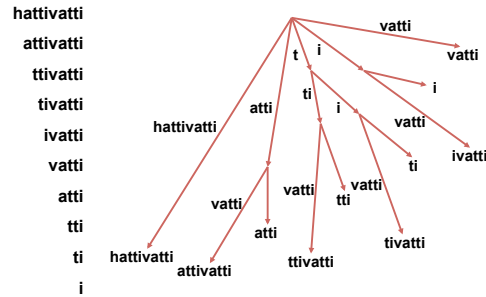
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Tree(T) is of linear size

- only the internal branching nodes and the leaves represented explicitly
- edges labeled by substrings of T
- $v = \text{node}(\alpha)$ if the path from root to v spells α
- one-to-one correspondence of leaves and suffixes
- $|T|$ leaves, hence $< |T|$ internal nodes
- $|\text{Tree}(T)| = O(|T| + \text{size}(\text{edge labels}))$

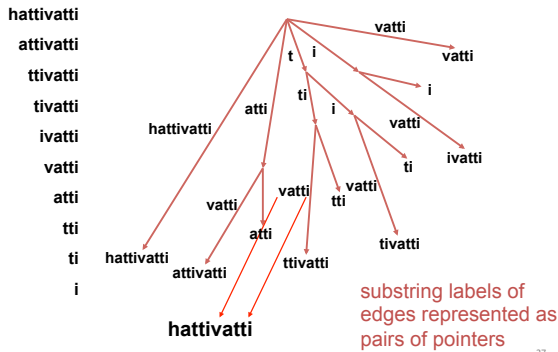
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Tree(hattivatti)



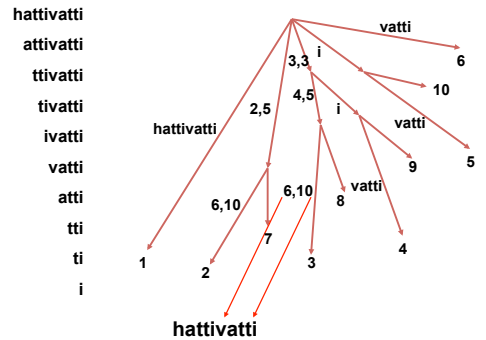
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Tree(hattivatti)



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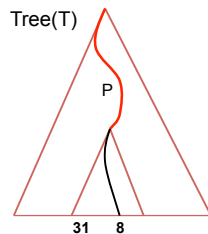
Tree(hattivatti)



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Tree(T) is full text index

P occurs in T at locations 8, 31, ...

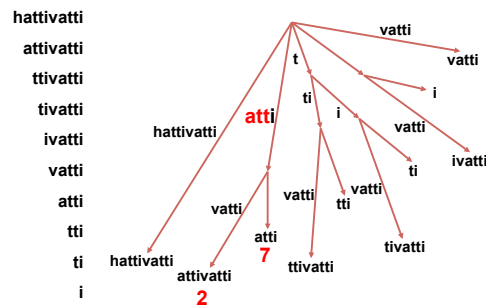


P occurs in T \Leftrightarrow P is a prefix of some suffix of T
 \Leftrightarrow Path for P exists in Tree(T)

All occurrences of P in time $O(|P| + \#\text{occ})$

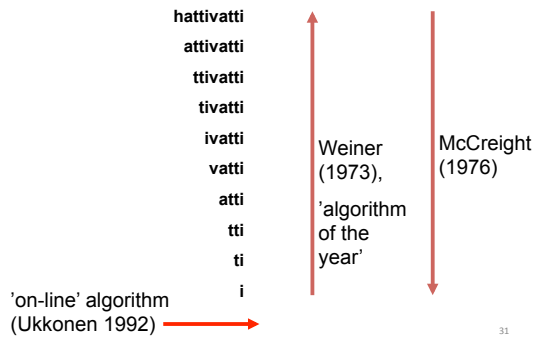
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Find att from Tree(hattivatti)



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Linear time construction of Tree(T)



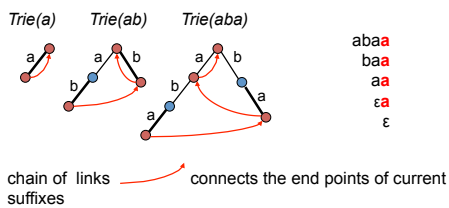
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On-line construction of Trie(T)

- $T = t_1 t_2 \dots t_n \$$
- $P_i = t_1 t_2 \dots t_i$ i :th prefix of T
- on-line idea: update $Trie(P_i)$ to $Trie(P_{i+1})$
- => very simple construction

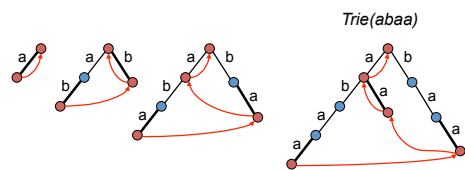
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Trie(abaab)



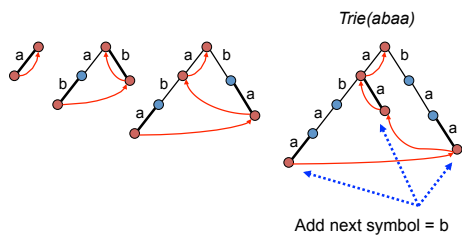
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Trie(abaab)



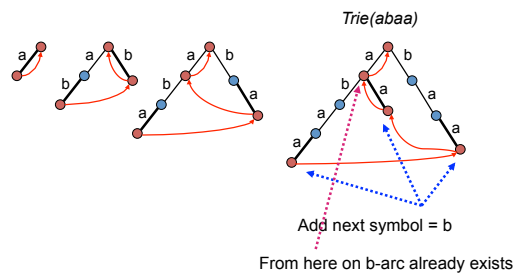
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Trie(abaab)

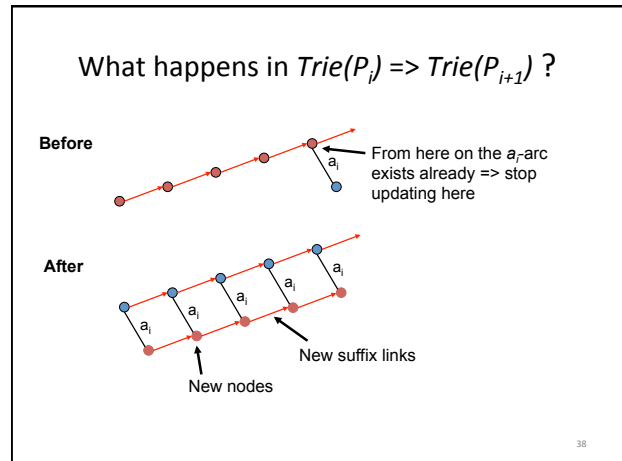
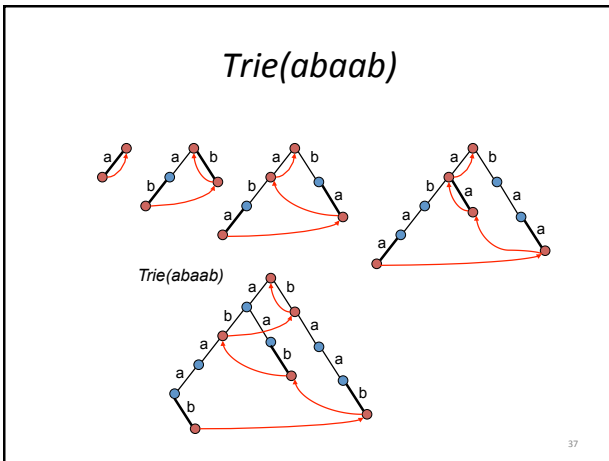


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Trie(abaab)



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What happens in $Trie(P_i) \Rightarrow Trie(P_{i+1})$?

- time: $O(\text{size of Trie}(T))$
- suffix links: slink
 $(\text{node}(a\alpha)) = \text{node}(\alpha)$

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On-line procedure for suffix trie

1. Create $Trie(t_i)$: nodes $root$ and v , an arc $son(root, t_i) = v$, and suffix links $slink(v) := root$ and $slink(root) := root$
2. **for** $i := 2$ to n **do begin**
3. $v_{p,i} :=$ leaf of $Trie(t_1 \dots t_{i-1})$ for string $t_1 \dots t_{i-1}$ (i.e., the deepest leaf)
4. $v := v_{p,i}; v' := 0$
5. **while** node v has no outgoing arc for t_i **do begin**
6. Create a new node v'' and an arc $son(v, t_i) = v''$
7. **if** $v' \neq 0$ **then** $slink(v) := v''$
8. $v := slink(v); v' := v''$ **end**
9. **for** the node v'' such that $v'' = son(v, t_i)$ **do**
if $v'' = v'$ **then** $slink(v') := root$ **else** $slink(v') := v''$

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Suffix trees on-line

- 'compact version' of the on-line trie construction: simulate the construction on the linear size tree instead of the trie => time $O(|T|)$
- all trie nodes are conceptually still needed => *implicit* and *real* nodes

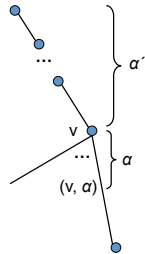
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Implicit and real nodes

- Pair (v, α) is an *implicit node* in $Tree(T)$ if v is a node of $Tree$ and α is a (proper) prefix of the label of some arc from v . If α is the empty string then (v, α) is a *'real'* node ($= v$).
- Let $v = \text{node}(\alpha')$ in $Tree(T)$. Then implicit node (v, α) represents $\text{node}(\alpha'\alpha)$ of $Trie(T)$

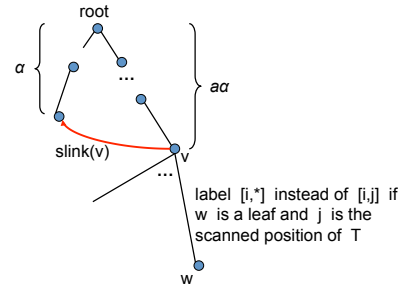
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Implicit node



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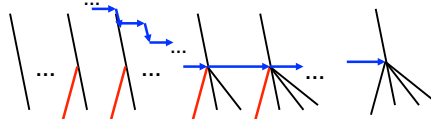
Suffix links and open arcs



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Big picture

suffix link path traversed: total work $O(n)$



new arcs and nodes created:
total work $O(\text{size}(\text{Tree}(T)))$

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On-line procedure for suffix tree

Input: string $T = t_1 t_2 \dots t_n \$$

Output: $\text{Tree}(T)$

Notation: $\text{son}(v, \alpha) = w$ iff there is an arc from v to w with label α

$\text{son}(v, \epsilon) = v$

Function $\text{Canonize}(v, \alpha)$:

while $\text{son}(v, \alpha') \neq 0$ where $\alpha = \alpha' \alpha'', |\alpha'| > 0$ **do**

$v := \text{son}(v, \alpha')$; $\alpha := \alpha''$

return (v, α)

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Suffix-tree on-line: main procedure

Create $\text{Tree}(t_1)$; $\text{slink}(\text{root}) := \text{root}$

$(v, \alpha) := (\text{root}, \epsilon)$ /* (v, α) is the start node */

for $i := 2$ **to** $n+1$ **do**

$v' := 0$

while there is no arc from v with label prefix at_i **do**

if $\alpha \neq \epsilon$ **then** /* divide the arc $w = \text{son}(v, \alpha\eta)$ into two */

$\text{son}(v, \alpha) := v''$; $\text{son}(v'', t_i) := v'''$; $\text{son}(v'', \eta) := w$

else

$\text{son}(v, t_i) := v'''$; $v''' := v$

if $v' \neq 0$ **then** $\text{slink}(v) := v''$

$v' := v''$; $v := \text{slink}(v)$; $(v, \alpha) := \text{Canonize}(v, \alpha)$

if $v' \neq 0$ **then** $\text{slink}(v) := v$

$(v, \alpha) := \text{Canonize}(v, at_i)$ /* (v, α) = start node of the next round */

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The actual time and space

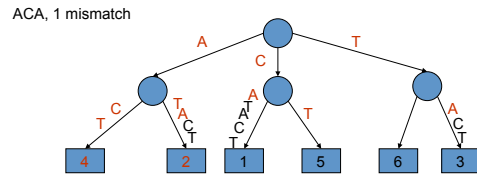
- $|\text{Tree}(T)|$ is about $20|T|$ in practice
- brute-force construction is $O(|T| \log |T|)$ for random strings as the average depth of internal nodes is $O(\log |T|)$
- difference between linear and brute-force constructions not necessarily large (Giegerich & Kurtz)
- truncated suffix trees: k symbols long prefix of each suffix represented (Na et al. 2003)
- alphabet independent linear time (Farach 1997)

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Applications of Suffix Trees

- **Dan Gusfield:** Algorithms on Strings, Trees, and Sequences: Computer Science and Computational Biology. Hardcover - 534 pages 1st edition (January 15, 1997). Cambridge Univ Pr (Short); ISBN: 0521585198. - book
- **APL1:** Exact String Matching Search for P from text S. Solution 1: build STree(S) - one achieves the same $O(n+m)$ as Knuth-Morris-Pratt, for example!
- Search from the suffix tree is $O(|P|)$
- **APL2:** Exact set matching Search for a set of patterns P

Back to backtracking



Same idea can be used to many other forms of approximate search, like Smith-Waterman, position-restricted scoring matrices, regular expression search, etc.

Applications of Suffix Trees

- **APL3:** substring problem for a database of patterns Given a set of strings $S=S_1, \dots, S_n$ --- a database Find all S_i that have P as a substring
- Generalized suffix tree contains all suffixes of all S_i
- Query in time $O(|P|)$, and can identify the LONGEST common prefix of P in all S_i

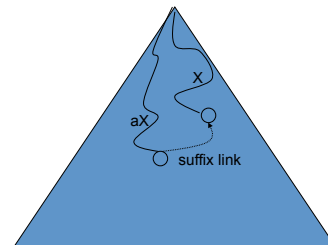
Applications of Suffix Trees

- **APL4:** Longest common substring of two strings
- Find the longest common substring of S and T.
- Overall there are potentially $O(n^2)$ such substrings, if n is the length of a shorter of S and T
- Donald Knuth once (1970) **conjectured** that linear-time algorithm is **impossible**.
- Solution: construct the STree(S+T) and find the node deepest in the tree that has suffixes from both S and T in subtree leaves.
- Ex: $S= superiorcalifornialives$ $T= sealiver$ have both a substring xxxxxx.

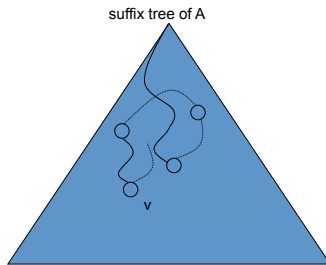
Simple analysis task: LCSS

- Let $LCSSA(A,B)$ denote the longest common substring two sequences A and B. E.g.:
 - $LCSS(AGATCTATCT,CGCCTCTATG)=TCTAT$.
- A good solution is to build suffix tree for the shorter sequence and make a *descending suffix walk* with the other sequence.

Suffix link

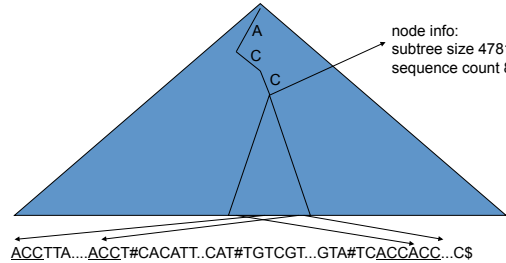


Descending suffix walk



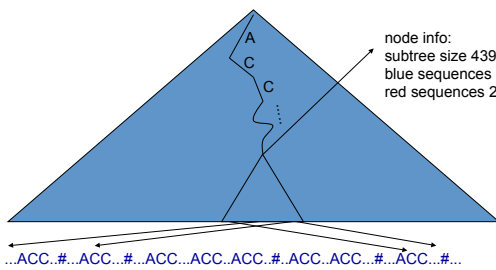
Read B left-to-right, always going down in the tree when possible. If the next symbol of B does not match any edge label on current position, take suffix link, and try again. (Suffix link in the root to itself emits a symbol). The node v encountered with largest string depth is the solution.

Another common tool: Generalized suffix tree



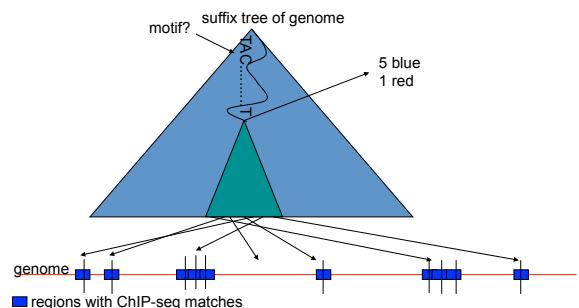
node info:
subtree size 47813871
sequence count 87

Generalized suffix tree application



node info:
subtree size 4398
blue sequences 12/15
red sequences 2/62

Case study continued



5 blue
1 red

Properties of suffix tree

- Suffix tree has n leaves and at most $n-1$ internal nodes, where n is the total length of all sequences indexed.
- Each node requires constant number of integers (pointers to first child, sibling, parent, text range of incoming edge, statistics counters, etc.).
- Can be constructed in linear time.

Properties of suffix tree... in practice

- Huge overhead due to pointer structure:
 - Standard implementation of suffix tree for human genome requires over **200 GB** memory!
 - A careful implementation (using $\log n$ -bit fields for each value and array layout for the tree) still requires over **40 GB**.
 - Human genome itself takes less than **1 GB** using 2-bits per bp.

Applications of Suffix Trees

- **APL4:** Longest common substring of two strings
- Find the longest common substring of S and T.
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- Donald Knuth once (1970) **conjectured** that linear-time algorithm is **impossible**.
- Solution: construct the $STree(S+T)$ and find the node deepest in the tree that has suffixes from both S and T in subtree leaves.
- Ex: S= *superiorcalifornialives* T= *sealiver* have both a substring *alive*.

Applications of Suffix Trees

- **APL5:** Recognizing DNA contamination Related to DNA sequencing, search for longest strings (longer than threshold) that are present in the DB of sequences of other genomes.
- **APL6:** Common substrings of more than two strings Generalization of APL4, can be done in linear (in total length of all strings) time

Applications of Suffix Trees

- **APL7:** Building a directed graph for exact matching: **Suffix graph** - directed acyclic word graph (DAWG), a **smallest finite state automaton** recognizing all suffixes of a string S. This automaton can recognize membership, but not tell which suffix was matched.
- Construction: merge isomorphic subtrees.
- Isomorphic in Suffix Tree when exists suffix link path, and subtrees have equal nr. of leaves.

Applications of Suffix Trees

- **APL8:** A reverse role for suffix trees, and major space reduction Index the pattern, not tree...
- Matching statistics.
- **APL10:** All-pairs suffix-prefix matching For all pairs S_p, S_q find the longest matching suffix-prefix pair. Used in shortest common superstring generation (e.g. DNA sequence assembly), EST alignment etc.

Applications of Suffix Trees

- **APL11:** Finding all maximal repetitive structures in linear time
- **APL12:** Circular string linearization e.g. circular chemical molecules in the database, one wants to linearize them in a canonical way...
- **APL13:** Suffix arrays - more space reduction will touch that separately

Applications of Suffix Trees

- **APL14:** Suffix trees in genome-scale projects
- **APL15:** A Boyer-Moore approach to exact set matching
- **APL16:** Ziv-Lempel data compression
- **APL17:** Minimum length encoding of DNA

Applications of Suffix Trees

- Additional applications Mostly exercises...
- Extra feature: **CONSTANT time lowest common ancestor retrieval (LCA)**
Andmestruktuur mis võimaldab leida konstantse ajaga alumist ühist vanemat (see vastab pikimale ühisele prefixile!) on võimalik koostada linearse ajaga.
- APL: Longest common extension: a bridge to inexact matching
- APL: **Finding all maximal palindromes in linear time**
Palindrome reads from central position the same to left and right. E.g.: kirik, saippuakivikauppias.
- Build the suffix tree of S and inverted S (aabcbad => aabcbad#dabcbaa) and using the LCA one can ask for any position pair (i, 2i-1), the longest common prefix in constant time.
- The whole problem can be solved in O(n).

Applications of Suffix Trees

- APL: Exact matching with wild cards
- APL: The k-mismatch problem
- Approximate palindromes and repeats
- Faster methods for tandem repeats
- A linear-time solution to the multiple common substring problem
- And many-many more ...

1. Suffix tree
2. **Suffix array**
3. Some applications
4. Finding motifs

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Suffixes - sorted

hattivatti	ε
attivatti	atti
ttivatti	attivatti
tivatti	hattivatti
ivatti	i
vatti	ivatti
atti	ti
tti	tivatti
ti	tti
i	ttivatti
ε	vatti

- Sort all suffixes. Allows to perform binary search!

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Suffix array: example

1	hattivatti	ε	11
2	attivatti	atti	7
3	ttivatti	attivatti	2
4	tivatti	hattivatti	1
5	ivatti	i	10
6	vatti	ivatti	5
7	atti	ti	9
8	tti	tivatti	4
9	ti	tti	8
10	i	ttivatti	3
11	ε	vatti	6

- suffix array = lexicographic order of the suffixes

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Suffix array construction: sort!

hattivatti	1	11
attivatti	2	7
ttivatti	3	2
tivatti	4	1
ivatti	5	10
vatti	6	5
atti	7	9
tti	8	4
ti	9	8
i	10	3
ε	11	6

- suffix array = lexicographic order of the suffixes

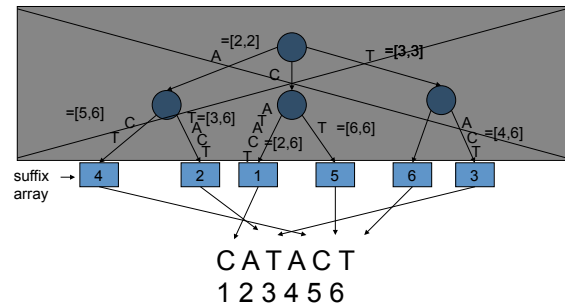
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Suffix array

- **suffix array** SA(T) = an array giving the lexicographic order of the suffixes of T
- space requirement: $5|T|$
- practitioners like suffix arrays (simplicity, space efficiency)
- theoreticians like suffix trees (explicit structure)

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Reducing space: suffix array



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Suffix array

- Many algorithms on suffix tree can be simulated using **suffix array**...
 - ... and couple of additional arrays...
 - ... forming so-called **enhanced suffix array**...
 - ... leading to the similar space requirement as careful implementation of suffix tree
- Not a satisfactory solution to the space issue.

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Pattern search from suffix array

hattivatti	ϵ	11	} att	binary search
attivatti	atti	7		
ttivatti	attivatti	2		
tivatti	hattivatti	1		
ivatti	i	10		
vatti	ivatti	5		
atti	ti	9		
tti	tivatti	4		
ti	tti	8		
i	ttivatti	3		
ϵ	vatti	6		

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What we learn today?

- We learn that it is possible to replace suffix trees with **compressed suffix trees** that take **8.8 GB** for the human genome.
- We learn that **backtracking** can be done using **compressed suffix arrays** requiring only **2.1 GB** for the human genome.
- We learn that **discovering** interesting motif seeds from the human genome takes **40 hours** and requires **9.3 GB** space.

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Recent suffix array constructions

- Manber&Myers (1990): $O(|T| \log |T|)$
- linear time **via suffix tree**
- January / June 2003: direct linear time construction of suffix array
 - Kim, Sim, Park, Park (CPM03)
 - Kärkkäinen & Sanders (ICALP03)
 - Ko & Aluru (CPM03)

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Kärkkäinen-Sanders algorithm

1. Construct the suffix array of the suffixes starting at positions $i \bmod 3 \neq 0$. This is done by reduction to the suffix array construction of a string of two thirds the length, which is solved recursively.
2. Construct the suffix array of the remaining suffixes using the result of the first step.
3. Merge the two suffix arrays into one.

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Notation

- string $T = T[0,n] = t_0 t_1 \dots t_{n-1}$
- suffix $S_i = T[i,0) = t_i t_{i+1} \dots t_{n-1}$
- for $C \subseteq [0,n]$: $S_C = \{S_i \mid i \in C\}$
- *suffix array* $SA[0,n]$ of T is a permutation of $[0,n]$ satisfying $S_{SA[0]} < S_{SA[1]} < \dots < S_{SA[n]}$

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Running example

- 0 1 2 3 4 5 6 7 8 9 10 11
- $T[0,n] = \text{y a b b a d a b b a d o o 0 0} \dots$
 - $SA = (12,1,6,4,9,3,8,2,7,5,10,11,0)$

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Step 0: Construct a sample

- for $k = 0,1,2$
 $B_k = \{i \in [0,n] \mid i \bmod 3 = k\}$
- $C = B_1 \cup B_2$ *sample positions*
- S_C *sample suffixes*
- Example: $B_1 = \{1,4,7,10\}$, $B_2 = \{2,5,8,11\}$, $C = \{1,4,7,10,2,5,8,11\}$

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Step 1: Sort sample suffixes

- for $k = 1,2$, construct
 $R_k = [t_k t_{k+1} t_{k+2}] [t_{k+3} t_{k+4} t_{k+5}] \dots [t_{\max B_k} t_{\max B_k+1} t_{\max B_k+2}]$

$R = R_1 \wedge R_2$ concatenation of R_1 and R_2

Suffixes of R correspond to S_C : suffix $[t_i t_{i+1} t_{i+2}] \dots$ corresponds to S_i ; correspondence is order preserving.

Sort the suffixes of R : radix sort the characters and rename with ranks to obtain R' . If all characters different, their order directly gives the order of suffixes. Otherwise, sort the suffixes of R' using Kärkkäinen-Sanders. Note: $|R'| = 2n/3$.

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Step 1 (cont.)

- once the sample suffixes are sorted, assign a rank to each: $\text{rank}(S_i) =$ the rank of S_i in S_C ; $\text{rank}(S_{n+1}) = \text{rank}(S_{n+2}) = 0$
- Example:
 $R = [\text{abb}][\text{ada}][\text{bba}][\text{do0}][\text{bba}][\text{dab}][\text{bad}][\text{o00}]$
 $R' = (1,2,4,6,4,5,3,7)$
 $SA_{R'} = (8,0,1,6,4,2,5,3,7)$ rank
 $(S_i) - 1\ 4 - 2\ 6 - 5\ 3 - 7\ 8 - 0\ 0$

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Step 2: Sort nonsample suffixes

- for each non-sample $S_i \in S_{B0}$ (note that rank (S_{i+1}) is always defined for $i \in B0$): $S_i \leq S_j \leftrightarrow (t_i, \text{rank}(S_{i+1})) \leq (t_j, \text{rank}(S_{j+1}))$
- radix sort the pairs $(t_i, \text{rank}(S_{i+1}))$.
- Example: $S_{12} < S_6 < S_9 < S_3 < S_0$ because $(0,0) < (a,5) < (a,7) < (b,2) < (y,1)$

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Step 3: Merge

- merge the two sorted sets of suffixes using a standard comparison-based merging:
- to compare $S_i \in S_C$ with $S_j \in S_{B0}$, distinguish two cases:
 - $i \in B1$: $S_i \leq S_j \leftrightarrow (t_i, \text{rank}(S_{i+1})) \leq (t_j, \text{rank}(S_{j+1}))$
 - $i \in B2$: $S_i \leq S_j \leftrightarrow (t_i, t_{i+1}, \text{rank}(S_{i+2})) \leq (t_j, t_{j+1}, \text{rank}(S_{j+2}))$
- note that the ranks are defined in all cases!
- $S_1 < S_6$ as $(a,4) < (a,5)$ and $S_3 < S_8$ as $(b,a,6) < (b,a,7)$

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Running time $O(n)$

- excluding the recursive call, everything can be done in linear time
- the recursion is on a string of length $2n/3$
- thus the time is given by recurrence

$$T(n) = T(2n/3) + O(n)$$
- hence $T(n) = O(n)$

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Implementation

- about 50 lines of C++
- code available e.g. via Juha Kärkkäinen's home page

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LCP table

- Longest Common Prefix of successive elements of suffix array:
- $\text{LCP}[i] =$ length of the longest common prefix of suffixes $S_{SA[i]}$ and $S_{SA[i+1]}$
- build inverse array SA^{-1} from SA in linear time
- then LCP table from SA^{-1} in linear time (Kasai et al, CPM2001)

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- [Oxford English Dictionary](http://www.oed.com/) <http://www.oed.com/>
- [Example - Word of the Day . Fourth](http://bits.cs.ut.ee/~vilo/edu/2005-06/Text_Algorithms/L7_SuffixTrees/wotd_fourth.html) <http://www.oed.com/cgi/display/wotd>
- PAT index - by **Gaston Gonnet** (ta on samuti Maple tarkvara üks loojatest ning hiljem molekulaarbioloogia tarkvarapaketi väljatöötajaid)
- PAT index is essentially a suffix array. To save space, indexed only from first character of every word
- XML-tagging (or SGML, at that time!) also indexed
- To mark certain fields of XML, the bit vectors were used.
- Main concern - improve the speed of search on the CD - minimize random accesses.
- For slow medium even 15-20 accesses is too slow...
- **G. H. Gonnet, R. A. Baeza-Yates**, and T. Snider, Lexicographical indices for text: Inverted files vs. PAT trees, Technical Report OED-91-01, Centre for the New OED, University of Waterloo, 1991.

Suffix tree vs suffix array

- suffix tree ↔ suffix array + LCP table

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1. Suffix tree
2. Suffix array
3. **Some applications**
4. Finding motifs

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Substring motifs of string T

- string $T = t_1 \dots t_n$ in alphabet A .
- Problem: **what are the frequently occurring (ungapped) substrings of T? Longest substring that occurs at least q times?**
- Thm: Suffix tree $Tree(T)$ gives complete occurrence counts of all substring motifs of T in $O(n)$ time (although T may have $O(n^2)$ substrings!)

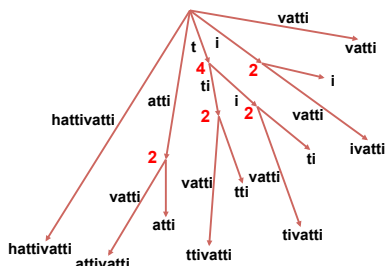
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Counting the substring motifs

- internal nodes of $Tree(T)$ ↔ repeating substrings of T
- number of leaves of the subtree of a node for string P = number of occurrences of P in T

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Substring motifs of hattivatti



Counts for the $O(n)$ maximal motifs shown

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Finding repeats in DNA

- human chromosome 3
- the first 48 999 930 bases
- 31 min cpu time (8 processors, 4 GB)
- Human genome: 3×10^9 bases
- $Tree(\text{HumanGenome})$ feasible

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Dynamic programming

$$d_{i,j} = \min(\text{if } a_i=b_j \text{ then } d_{i-1,j-1} \text{ else } \infty, d_{i-1,j} + 1, d_{i,j-1} + 1)$$

= distance between i-prefix of A and j-prefix of B (substitution excluded)

mxn table d

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$$d_{i,j} = \min(\text{if } a_i=b_j \text{ then } d_{i-1,j-1} \text{ else } \infty, d_{i-1,j} + 1, d_{i,j-1} + 1)$$

A\B		s	t	o	c	k	h	o	l	m
	0	1	2	3	4	5	6	7	8	9
t	1	2	1	2	3	4	5	6	7	8
u	2	3	2	3	4	5	6	7	8	9
k	3	4	3	4	5	4	5	6	7	8
h	4	5	4	5	6	5	4	5	6	7
o	5	6	5	4	5	6	5	4	5	6
l	6	7	6	5	6	7	6	5	4	5
m	7	8	7	6	7	8	7	6	5	4
a	8	9	8	7	8	9	8	7	6	5

optimal alignment by trace-back $d_D(A,B)$

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Search problem

- find approximate occurrences of pattern P in text T: substrings P' of T such that d(P,P') small
- dyn progr with small modification: O(mn)
- lots of (practical) improvement tricks

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Index for approximate searching?

- dynamic programming: P x Tree(T) with backtracking

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- Suffix tree
- Suffix array
- Some applications
- Finding motifs**

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Gapped motifs

a##bc

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Gapped motifs

a##bc a##bc
 ababbccbc**aa**abca

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Gapped motifs of T

- **gapped pattern**: P in $(A \cup \{\#\})^*$
- **gap symbol** $\#$ matches any symbol in A
- $aa##bb#b$
- $L(P)$ = occurrence locations of P in T
- P is called a **motif** of T if $|L(P)| > 1$ and a motif with **quorum** q if $|L(P)| \geq q$.
- **Problem**: find occurrence count $|L(P)|$ for all gapped motifs P of T
- $a^n b a^n$ has exponentially many motifs!

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Maximal motifs

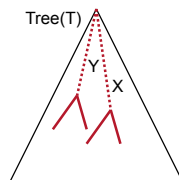
- motif P' is the **maximal version** of motif P if P' has the largest possible number of non- $\#$ symbols among motifs that have the same set of occurrence locations as P
- every motif has unique maximal version
- unfortunately still exponential number of different maximal motifs

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Blocks of maximal motifs

- $aaa##b##ba$ has **blocks** aaa, b, ba
- **Lemma**: Maximal 1-block motifs \leftrightarrow (branching) nodes of $Tree(S)$
- **Thm**: Each block of a maximal motif of T is a maximal substring motif of T . Hence there are $O(n)$ different strings that can be used as a block of a maximal motif.
- \Rightarrow There are $O(n^{2^{k-1}})$ different maximal motifs with k blocks [$O(n^{2^k})$ unrestricted motifs].

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Two-block maximal pattern: $X###Y$

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Counting 2-block maximal motifs

- **Thm**: The occurrence counts for all maximal motifs with two blocks can be found in (optimal) time $O(n^3)$.
- c.f., Arimura et al (2000), Apostolico et al (2004), ...

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Algorithm (very simple)



for each maximal substring motif X
 for each distance $d = 1, 2, \dots$
 mark the leaves of $Tree(T)$ that correspond to locations $L(X) + d$
 for each maximal substring motif Y ,
 find the number $h(Y)$ of marked leaves in its subtree in $Tree(T)$
 the occurrence count of motif (X,d,Y) is $h(Y)$

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Algorithm (very simple)



for each maximal substring motif X $O(n)$
 for each distance $d = 1, 2, \dots$ $O(n)$
 mark the leaves of $Tree(T)$ that correspond to locations $L(X) + d$ $O(n)$
 for each maximal substring motif Y ,
 find the number $h(Y)$ of marked leaves in its subtree in $Tree(T)$
 the occurrence count of motif (X,d,Y) is $h(Y)$

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Counting 2-block maximal motifs (cont)

- Thm: The occurrence counts for all maximal motifs with two blocks can be found in (optimal) time $O(n^3)$.
- flexible gaps:
 x^*y $*$ = gap of any length
- Thm: The occurrence counts for all maximal motifs with two blocks and one flexible gap can be found in (optimal) time $O(n^2)$.
- k-block case?

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Conclusion

- suffix structures provide very efficient algorithmic tools for finding and learning potentially interesting patterns in strings

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General case

- Q1: Given q and W , has T a motif with at least W non-gap symbols and at least q occurrences?
- In k-block case, is $O(n^{2k-1})$ (or even better) time possible?
- related work: H.Arimura&al, A. Apostolico &al, M-F. Sagot, L. Parida, N. Pisanti, ...

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