Regularities in Sequences

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joint work with

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German Cancer Research Center, Heidelberg, Germany

Chennai, December 1999

Regularities in Sequences

or a longer title...

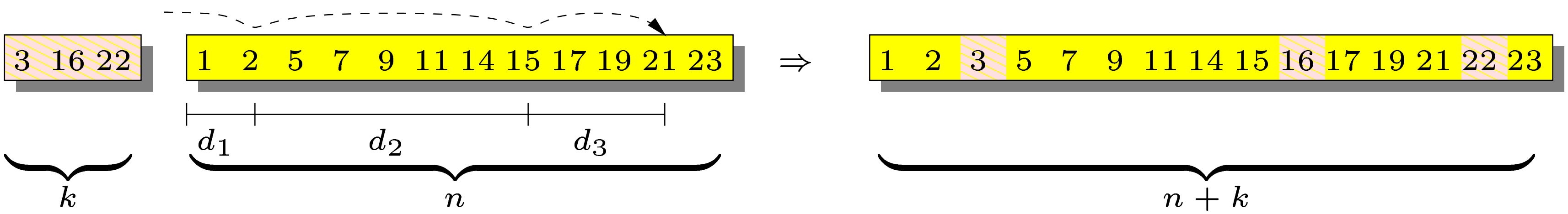
On Using Efficient Merging in $\mathcal{O}(n \log n)$ Time Algorithms for Finding Regularities in Strings

Merging $\rightarrow$ $\mathcal{O}(n \log n)$ Algorithms $\rightarrow$ Strings $\rightarrow$ Regularities

Comparison Based Merging

Problem

Merge two sorted sequences of length k and n, $k \leq n$



Solutions

(1) Sequential merging $\Rightarrow \mathcal{O}(n+k)$ comparisons

(2) Merging using exponential searching $\Rightarrow$

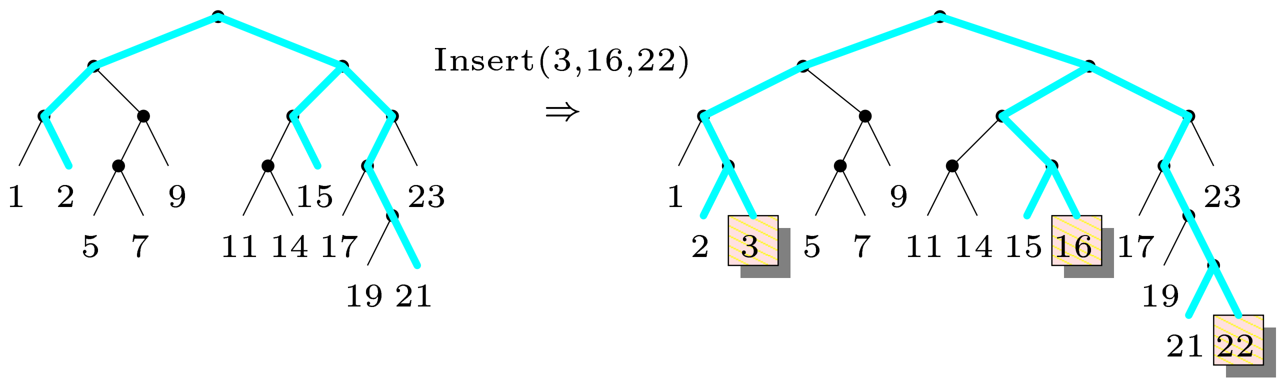
$$\Theta\left(\sum_{i=1}^{k} \log d_i\right) = \Theta\left(\log \binom{n+k}{k}\right) \text{ comparisons}$$

Hwang & Lin 1972

Time ?

Merging Search Trees

Brown & Tarjan 1979



Merging two balanced search trees of size k and n, $k \leq n$

- Size k tree ⇒ list of k elements $\mathcal{O}(k)$
- Search for the k elements in **one traversal** of the size n tree $\mathcal{O}\left(\left|\bigcup_{i=1}^{k} \text{search-path}_i\right|\right)$
- Insert the k elements $\mathcal{O}(k)$
- Rebalance typically amortized $\mathcal{O}(k)$

$\bigcup$ paths ?

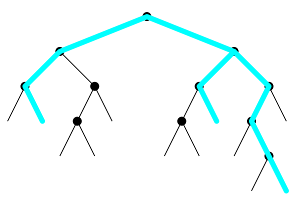
Path Theorem

Brown & Tarjan 1979

Theorem

In a **balanced** search tree with n leaves the #edges in the union of k distinct root-to-leaf paths is

$$\left| \bigcup_{i=1}^{k} \text{path}_i \right| = \mathcal{O}\left(\log \binom{n+k}{k}\right)$$



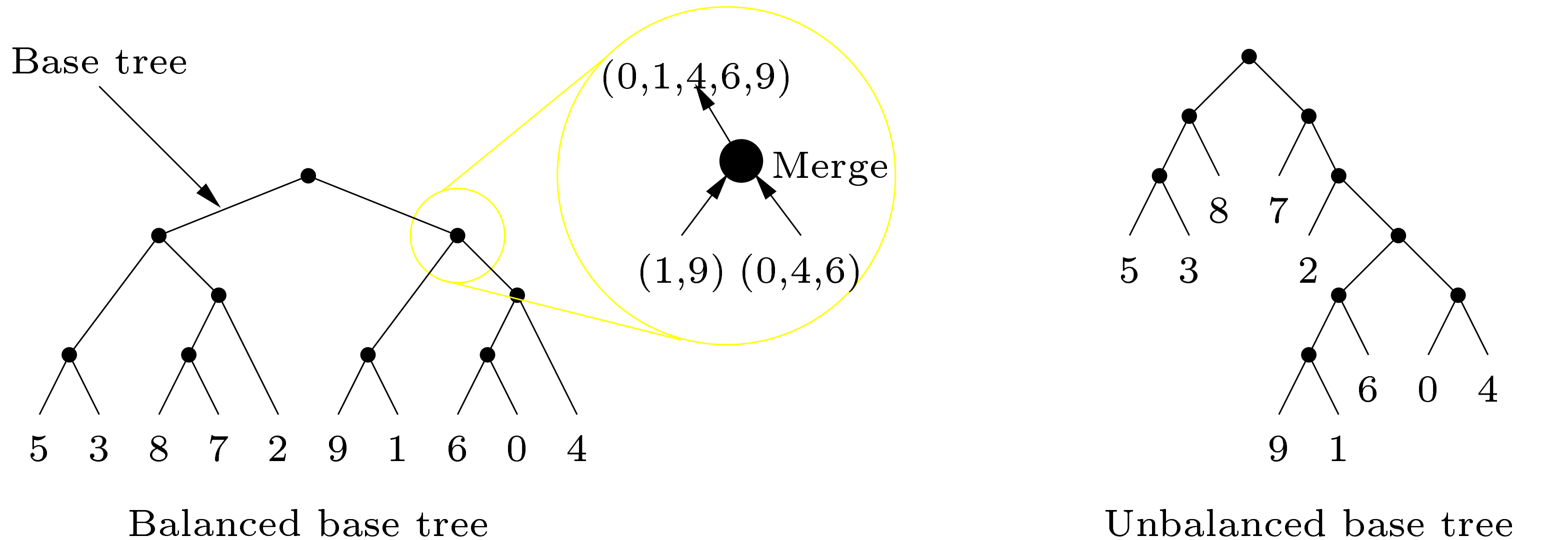
[e.g. AVL–trees, red–black trees, 2–3–trees, 2–4–trees, ...]

Corollary

Merging two trees of size k and n, $k \leq n$, takes time $\mathcal{O}\left(\log \binom{n+k}{k}\right)$ which is optimal

Merge Sort ?

Merge Sort — Revisited



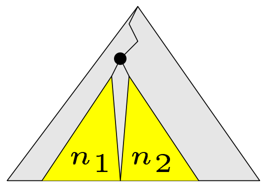
Balanced base tree	+	Sequential merging	$\Rightarrow$	$\mathcal{O}(n \log n)$
Unbalanced base tree	+	Sequential merging	$\Rightarrow$	$\mathcal{O}(n^2)$
Unbalanced base tree	+	Merging by insertion*	$\Rightarrow$	$\mathcal{O}(n \log^2 n)$
Unbalanced base tree	+	Optimal merging	$\Rightarrow$	$\mathcal{O}(n \log n)$

$n \log n$?

Merge Sort — Analysis

Theorem

If we spend time $\mathcal{O}\left(\log\binom{n_1+n_2}{n_1}\right)$ at each node with two children spanning respectively n_1 and n_2 leaves, $n_1 \leq n_2$, then we in a subtree spanning n leaves spend total time $\mathcal{O}(\log n!)$



Proof

Induction, using

$$\begin{aligned}
&\log n_1! + \log n_2! + \log\binom{n_1+n_2}{n_1} \\
&= \log n_1! + \log n_2! + \log\frac{(n_1+n_2)!}{n_1!\cdot n_2!} \\
&= \log n_1! + \log n_2! + \log(n_1+n_2)! - \log n_1! - \log n_2! \\
&= \log(n_1+n_2)!
\end{aligned}$$

□

Corollary

Merging n singleton lists using any base tree takes time $\mathcal{O}(n\log n)$

Applications of the Path Lemma

Searching

Searching for the predecessors of $e_1 \leq \cdots \leq e_k$ in a balanced search tree of size $n \geq k$ takes time $\mathcal{O}\left(\log \binom{n+k}{k}\right)$

Δ–Searching

The δ-predecessor of an x in a sorted list $L = (x_1, \ldots, x_n)$ is defined by

$$\begin{aligned} \text{max-gap}(L) &= \max\{0, x_2 - x_1, \ldots, x_n - x_{n-1}\} \\ \Delta\text{-pred}(L, \delta, x) &= \min\{y \in L \mid \text{max-gap}(L \cap [y, x]) \leq \delta\} \end{aligned}$$

Ex. $\Delta\text{-pred}(\ (1, 2, \underline{5, 7, 9, 11}, 14, 15, 17, 19, 21, 23),\ 2,\ 13\ ) = 5$

- Multi-Δ-Pred$(T, \delta, e_1, \ldots, e_k)$ for each e_i finds $\Delta\text{-pred}(T, \delta, e_i)$

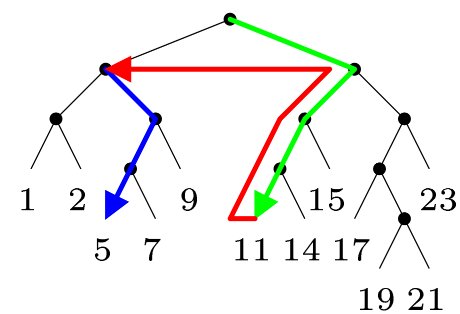
Δ-Pred ?

Δ–Searching

For each node v store $\min(T_v)$, $\max(T_v)$, and max-gap(T_v)

The computation of Δ-pred(T, δ, e) proceeds in three phases

- compute pred(T, e)
- search for Δ-pred$(T, \delta, \min(T_v))$
- search for Δ-pred$(T_v, \delta, \max(T_v))$



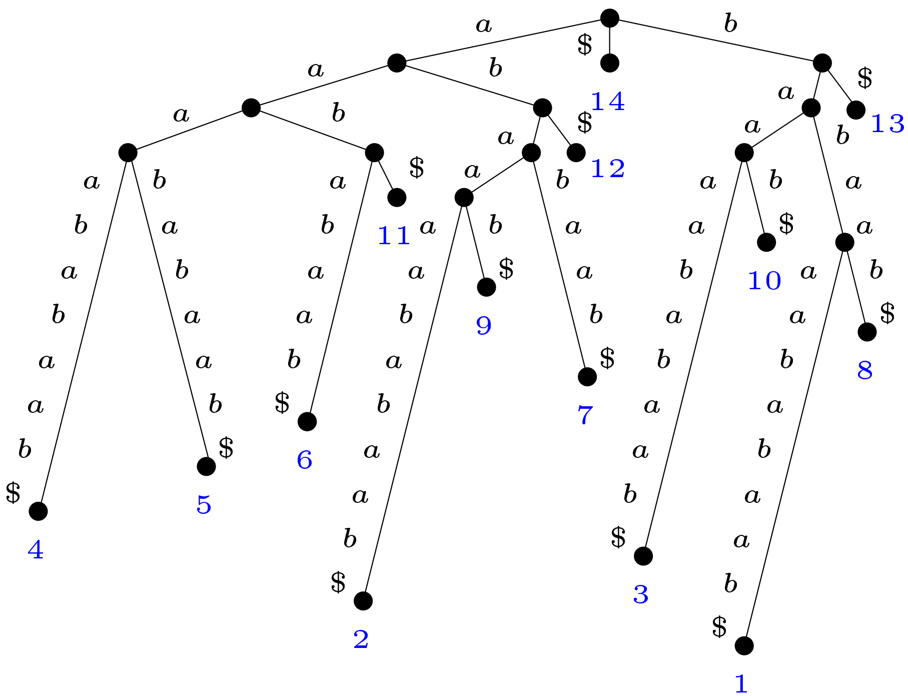
Δ-pred(T, 2, 13)

Multi-Δ-Pred$(T, \delta, e_1, \ldots, e_k)$ can be performed in time $\mathcal{O}\left(\log \binom{n+k}{k}\right)$ when $e_1 \leq \cdots \leq e_k$ and $k \leq n$, e.g. using dynamic programing to only compute Δ-pred$(T, \delta, \min(T_v))$ and Δ-pred$(T, \delta, \max(T_v))$ once per node

String Notation

Notation		Example		
Alphabet	Σ	Σ	$=$	$\{a, b\}$
String	$S \in \Sigma^*$	S	$=$	$b\,a\,b\,a\,a\,a\,a\,b\,a\,b\,a\,a\,b$
ith character	$S[i]$	$S[3]$	$=$	b
Substring	$S[i\,..\,j]$	$S[3\,..\,8]$	$=$	$b\,a\,a\,a\,a\,b$
Occurrence	(α, i)	$(\,b\,a\,b\,,\,8\,)$	$=$	$b\,a\,b\,a\,a\,a\,a\,\underline{b\,a\,b}\,a\,a\,b$
Tandem repeat	$\alpha\alpha$	$\alpha\alpha$	$=$	$\underline{b\,a}\,\underline{b\,a}$
Pair	(α, i, j)	$(\,b\,a\,b\,a\,,\,1,\,8\,)$	$=$	$\underline{b\,a\,b\,a}\,a\,a\,a\,\underline{b\,a\,b\,a}\,a\,b$

Suffix Trees



$S = b\,a\,b\,a\,a\,a\,a\,b\,a\,b\,a\,a\,b$

Suffixes

$b\,a\,b\,a\,a\,a\,a\,b\,a\,b\,a\,a\,b\,\$$
$a\,b\,a\,a\,a\,a\,b\,a\,b\,a\,a\,b\,\$$
$b\,a\,a\,a\,a\,b\,a\,b\,a\,a\,b\,\$$
$a\,a\,a\,a\,b\,a\,b\,a\,a\,b\,\$$
$a\,a\,a\,b\,a\,b\,a\,a\,b\,\$$
$a\,a\,b\,a\,b\,a\,a\,b\,\$$
$a\,b\,a\,b\,a\,a\,b\,\$$
$b\,a\,b\,a\,a\,b\,\$$
$a\,b\,a\,a\,b\,\$$
$b\,a\,a\,b\,\$$
$a\,a\,b\,\$$
$a\,b\,\$$
$b\,\$$
$\$$

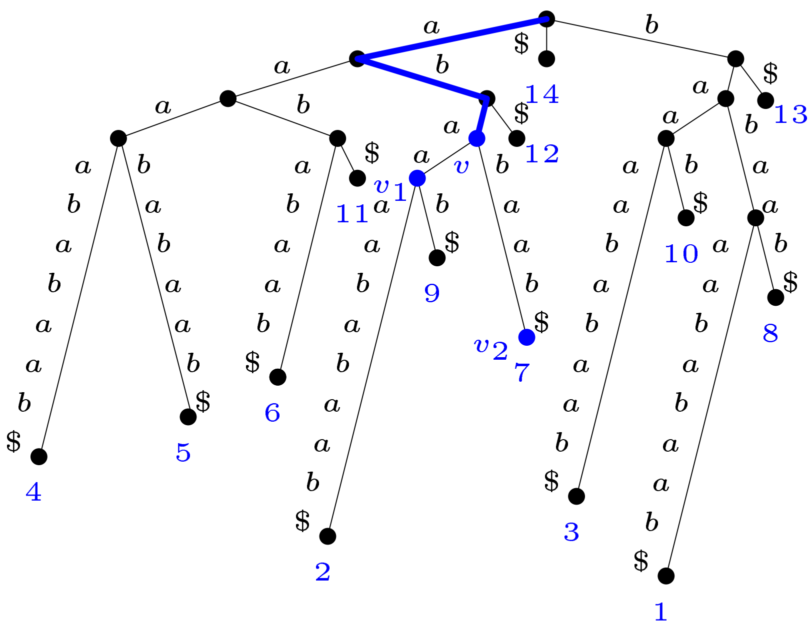
Suffix tree of S $\equiv$ trie of all suffixes of $S\$$, where $\$ \notin \Sigma$

Leaf labeled i $\equiv$ suffix $S[i\,..]\$$

Theorem

The suffix tree of S can be constructed in time $\mathcal{O}(n)$ — Weiner 1973

Path Labels and Leaf Lists



$S = b\,\underline{a\,b\,a}\,a\,a\,\underline{a\,b\,\underline{a}}\underline{\,b\,a}\,a\,b$
$L(v) = a\,b\,a$
$LL(v_1) = \{2, 9\}$
$LL(v_2) = \{7\}$
$LL(v) = LL(v_1) \cup LL(v_2) = \{2, 7, 9\}$

Let v be a node in the suffix tree of S

Path-label $L(v)$ = string spelled from the root to v

Leaf-list $LL(v)$ = set of leaf labels in the subtree rooted at v

$$LL(v) = \text{all occurrences of } L(v) = \bigcup_{c \in \text{children}(v)} LL(c)$$

Regularities

We will develop $\mathcal{O}(n \log n + |\text{output}|)$ time algorithms for

- Finding all tandem repeats in S

$$b\,a\,b\,a\,a\,a\,a\,\underline{b\,a}\,\underline{b\,a}\,a\,b$$

- Finding all maximal pairs in S with bounded gap

$$\underline{b\,a\,b\,a\,a}\,\underbrace{a\,a}_{\text{gap}}\,\underline{b\,a\,b\,a\,a}\,b$$

- Finding all maximal quasi-periodic substrings in S

$$a\,a\,a\,b\,a\,a\,b\,b\,b\,\overline{a\,b\,a\,a\,b\,a\,a\,b\,a\,a\,b\,a\,a}\,b\,b\,a\,a\,a\,b\,a$$

Tandem Repeats

Stoye & Gusfield 1998

Problem

Given S, find all substrings of S which are tandem repeats

For each tandem repeat occurrence $(\alpha\alpha, i)$ output $(|\alpha|, i)$

Ex. $S = b\,a\,b\,a\,a\,a\,a\,b\,a\,b\,a\,a\,b$

Output $= (2,1), (1,4), (1,5), (1,6), (2,7), (2,8), (1,11)$

Tandem repeat occ. $(|\alpha|, i)$ is branching iff $S[i + |\alpha|] \neq S[i + 2|\alpha|]$

Ex. $(2,7)$ is non-branching and $(2,8)$ is branching

$(|\alpha|, i)$ non-branching $\Rightarrow$ $(|\alpha|, i+1)$ tandem repeat occ.

Given all branching tandem repeat occ. we can compute all tandem repeat occ. in time $\mathcal{O}(|\text{output}|)$

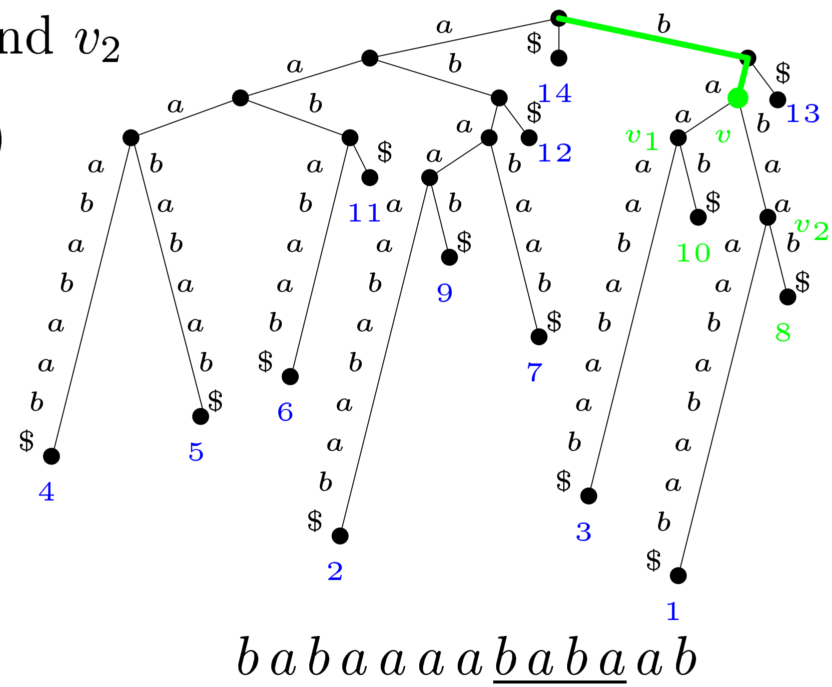
Branching ?

Branching Tandem Repeat Occurrences

Lemma

$(\alpha\alpha, i)$ is a branching tandem repeat occurrence in S iff

- $\exists$ node v in the suffix tree of S with $L(v) = \alpha$
- v has two distinct children v_1 and v_2
- $i \in LL(v_1)$ and $i + |\alpha| \in LL(v_2)$



Branching Tandem Repeat Occurrences

Algorithm

1. Compute suffix tree (w.l.o.g. all nodes $\leq$ two children) $\mathcal{O}(n)$
2. Bottom-up do for each node v with children v_1 and v_2
   $n_1 = |LL(v_1)| \leq |LL(v_2)| = n_2$

   a) For each $i \in LL(v_1)$ search for $i \pm |L(v)|$ in $LL(v_2)$
      using optimal multi-search $\mathcal{O}\left(\log \binom{n_1+n_2}{n_1}\right)$
      If $i + |L(v)| \in LL(v_2)$ then output $(|L(v)|, i)$
      If $i - |L(v)| \in LL(v_2)$ then output $(|L(v)|, i - |L(v)|)$

   b) $LL(v) = LL(v_1) \cup LL(v_2)$
      using optimal tree merging $\mathcal{O}\left(\log \binom{n_1+n_2}{n_1}\right)$

Total time $\mathcal{O}(n \log n)$, i.e. $\mathcal{O}(n \log n)$ branching tandem repeat occ.

Maximal Pairs with Bounded Gap

Brodal et al. 1999

A pair (α, i, j) is

- right-maximal iff $S[i+|\alpha|] \neq S[j+|\alpha|]$
- left-maximal iff $S[i-1] \neq S[j-1]$
- maximal iff both right- and left-maximal

The gap of $(\alpha, i, j) = \max(i,j) - \min(i,j) - |\alpha|$

Ex. $b\, \underline{\underline{a\, b}\, a}\, a\, a\, \underline{\underline{a\, b}\, a}\, b\, a\, a\, b$

$(a\, b, 2, 7)$ is left-maximal but not right-maximal

$(a\, b\, a, 2, 7)$ is maximal and gap $= 2$

Problem

Given S, find all maximal pairs in S with gap in an interval $[\Delta_L, \Delta_H]$

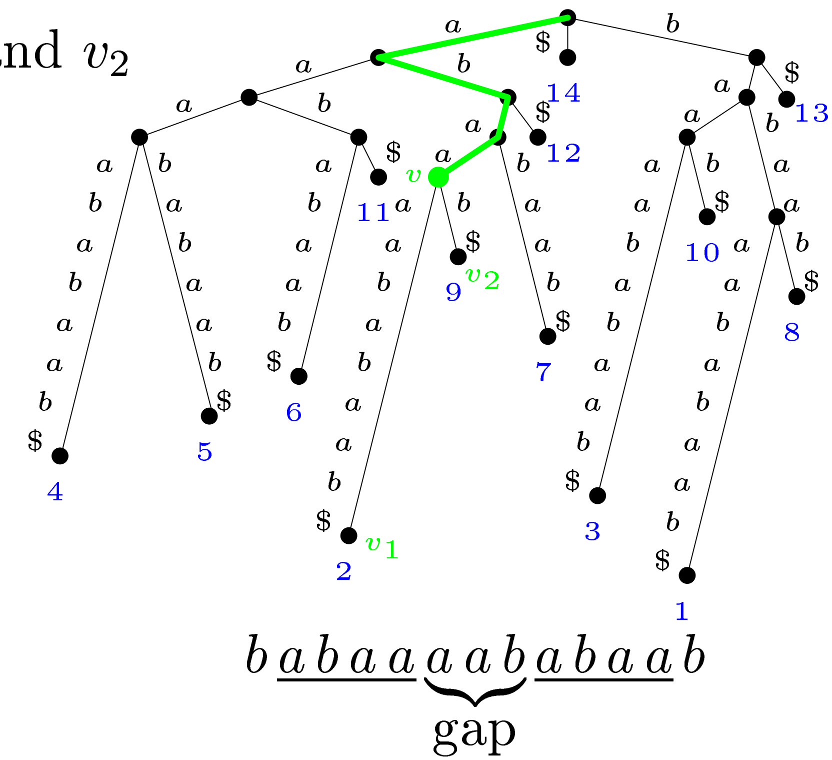
For each such pair (α, i, j) output $(|\alpha|, i, j)$

Right-Maximal Pairs

Lemma

(α, i, j) is a right-maximal pair in S iff

- $\exists$ node v in the suffix tree of S with $L(v) = \alpha$
- v has two distinct children v_1 and v_2
- $i \in LL(v_1)$ and $j \in LL(v_2)$



Right-Maximal Pairs with Bounded Gap

Algorithm

1. Compute suffix tree (w.l.o.g. all nodes $\leq$ two children) $\mathcal{O}(n)$
2. Bottom-up do for each node v with children v_1 and v_2
   $n_1 = |LL(v_1)| \leq |LL(v_2)| = n_2$

   a) For each $i \in LL(v_1)$ search for $i \pm (|L(v)| + \Delta_H)$ in $LL(v_2)$ $\mathcal{O}\left(\log \binom{n_1+n_2}{n_1}\right)$

   $j \in [i{+}|L(v)|{+}\Delta_L \,..\, i+|L(v)|{+}\Delta_H] \cap LL(v_2)$ output $(|L(v)|, i, j)$

   $j \in [i{-}|L(v)|{-}\Delta_H \,..\, i-|L(v)|{-}\Delta_L] \cap LL(v_2)$ output $(|L(v)|, j, i)$

   $\mathcal{O}(|\text{output}|)$

   b) $LL(v) = LL(v_1) \cup LL(v_2)$ $\mathcal{O}\left(\log \binom{n_1+n_2}{n_1}\right)$

Total time $\mathcal{O}(n \log n + |\text{output}|)$ Maximal ?

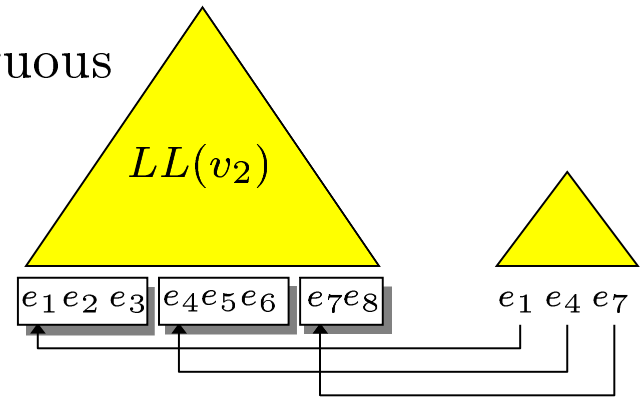
Maximal Pairs with Bounded Gap

Simple approach

- Compute all right-maximal pairs $(|\alpha|, i, j)$ with bounded gap
- Output all $(|\alpha|, i, j)$ where $S[i-1] \neq S[j-1]$

... but requires too much time

Efficient approach



Divide the leaf-lists into blocks of contiguous indices with same left-character

For each $LL(v)$ keep a tree with the starting points of each block

In the computation of

$$\{j \in [i+|L(v)|+\Delta_L .. i+|L(v)|+\Delta_H] \cap LL(v_2) \ : \ S[j-1] \neq S[i-1]\}$$

a block of j's where $S[j-1] = S[i-1]$ can be skipped in time $\mathcal{O}(1)$

Total time $\mathcal{O}(n \log n + |\text{output}|)$

Maximal Quasi-Periodic Substrings

A string is quasi-periodic if it can be covered by a shorter substring

$$a\,b\,a\,a\,b\,a\,a\,b\,a\,a\,b\,a\,a\,b$$

$S[i\,..\,j]$ is a maximal quasi-periodic substring with quasi-period α iff

- α is not quasi-periodic and α covers $S[i\,..\,j]$
- no extension of $S[i\,..\,j]$ is covered by α
- $\alpha\, S[j+1]$ does not cover $S[i\,..\,j+1]$

$$S[i\,..\,j]$$

$$a\,a\,a\,b\,a\,a\,b\,b\,b\,a\,b\,a\,a\,b\,a\,a\,b\,a\,a\,b\,a\,a\,b\,b\,a\,a\,a\,b\,a$$

$$\alpha$$

Problem

Find all $(|\alpha|, i, j)$ where $S[i\,..\,j]$ is a maximal quasi-periodic substring with quasi-period α

Apostolico & Ehrenfeucht 1993

$\mathcal{O}(n \log^2 n)$

Maximal Quasi-Periodic Substrings

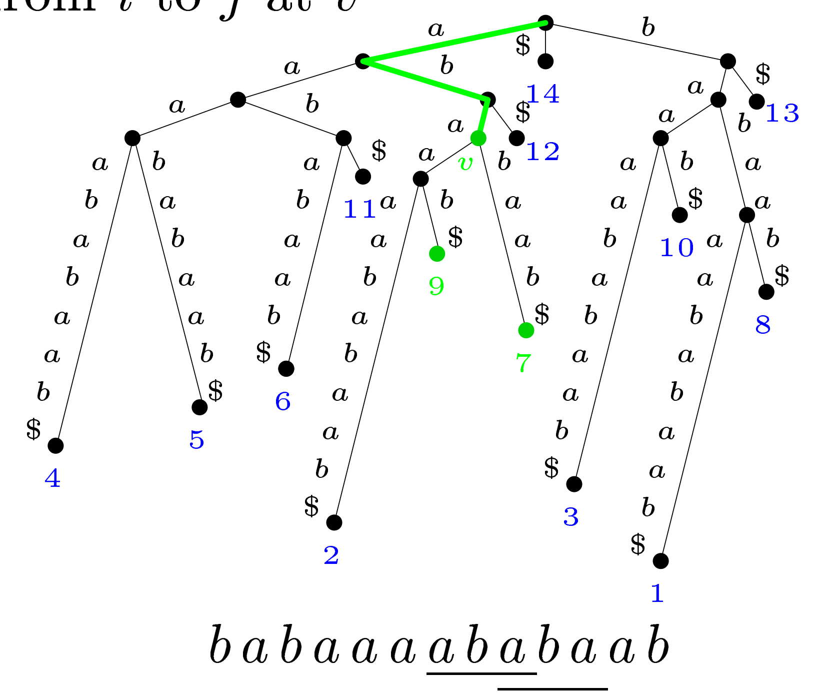
Theorem

$(|\alpha|, i, j)$ is a maximal quasi-periodic substring of S iff

1. There exists a node v in the suffix tree of S with $L(v) = \alpha$
2. The $L(v)$ is not quasi-periodic
3. There exists a coalescing run from i to j at v

A run is a maximal subsequence of adjacent or overlapping occurrences of $L(v)$ in $LL(v)$

A coalescing run is a run containing indices from leaf-lists of two children of v



Finding Maximal Quasi-Periodic Substrings

Algorithm

1. Mark all v where $L(v)$ not quasi-periodic $\mathcal{O}(n \log n)$

   The most complicated step — applies multi-searches and merging

2. Bottom-up do for each node v with children v_1 and v_2

   $n_1 = |LL(v_1)| \leq |LL(v_2)| = n_2$

   a) Compute $LL(v) = LL(v_1) \cup LL(v_2)$ $\mathcal{O}\left(\log \binom{n_1+n_2}{n_1}\right)$

   b) For each coalescing run in $LL(v)$ identify at least one $i \in LL(v_1)$ in the run $\mathcal{O}(n_1)$

   c) Apply $\textsf{Multi-}\Delta\textsf{-Pred}(LL(v), |L(v)|, \ldots)$ to the result of b) to find the start and end of each coalescing run $\mathcal{O}\left(\log \binom{n_1+n_2}{n_1}\right)$

   d) If v is marked then report all the coalescing runs found in c) as maximal quasi-periodic substrings

Total time $\mathcal{O}(n \log n)$, i.e. $\mathcal{O}(n \log n)$ maximal quasi-periodic substrings

Theorems Applied

Theorem

In a **balanced** search tree with n leaves the #edges in the union of k distinct root-to-leaf paths is

$$\left|\bigcup_{i=1}^{k} \text{path}_i\right| = \mathcal{O}\left(\log \binom{n+k}{k}\right)$$

Theorem

If we spend time $\mathcal{O}\left(\log \binom{n_1+n_2}{n_1}\right)$ at each node with two children spanning respectively n_1 and n_2 leaves, $n_1 \leq n_2$, then we in a subtree spanning n leaves spend total time $\mathcal{O}(\log n!)$

Conclusion

- We have presented $\mathcal{O}(n \log n + |\text{output}|)$ time algorithms for finding all tandem repeats, maximal pairs with bounded gap, and maximal quasi-periodic substrings of a string
- Based on efficient merging and two related theorems
- The data structuring approach allowed us to concentrate on a few crucial underlying string properties

Open problem

- Can the time be improved to $o(n \log n)$ for finding all pairs with bounded gap or all maximal quasi-periodic substrings ?

Without an upper bound on the gaps all pairs can be found in time $\mathcal{O}(n + |\text{output}|)$ Brodal et al. 1999

A compact representation of all tandem repeats can be found in time $\mathcal{O}(n)$ Gusfield & Stoye 1998