UNIVERSITÄT DES SAARLANDES

ZBI ZENTRUM FÜR BIOINFORMATIK

Suffix Trees

Algorithms for Sequence Analysis

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Motivation

What have we learned so far

Algorithms for $O(n+m)$ pattern search,
for a pattern P of length m and text T of length n

Observation: $m \ll n$ in many applications

- mapping millions of sequenced DNA fragments to the human genome ($n > 3 \cdot 10^9$ bp)
- full text search on websites, forums, etc.
- finding motifs in a large set of sequences

Idea

Build an **index** over the text first to allow very fast searches in $O(m)$ time
Today: Suffix tries and trees

Motivation: Runtimes

	online search	**index-based search**
Preprocessing	$O(m)$	$O(n)$
Search one pattern	$O(n)$	$O(m)$
Preprocess and search k patterns	$O\big(k(m+n)\big)$	$O\big(n+km\big)$

Trees

- A **rooted tree** is a connected acyclic graph with a special node r, the **root node**, such that all edges point away from the root.
- The **depth** $depth(v)$ of a node v is its distance from the root; i.e. the number of edges on the unique path from the root to v. In particular, $depth(r) = 0$.

Edge-labeled Trees

- **Σ-tree** or **trie**: rooted tree whose edges are each annotated with one single letter from Σ, such that no node has two outgoing edges labeled with the same letter.

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- tree is **compact** if no node (other than possibly root r) has exactly one child.
- node with no outgoing edges is called **leaf**.

Black board: Edge-labeled Trees

Suffix Trees

- A Σ-tree or Σ^+-tree T **spells** $x \in \Sigma^*$ if x can be read along a path starting from root.
- *words*(T): set of strings spelled by T.

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$words(T) = \{s' \mid s' \text{ is a substring of } s\}$.

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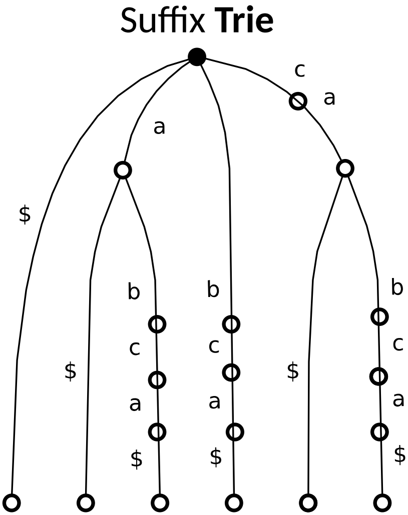
Sentinel Character

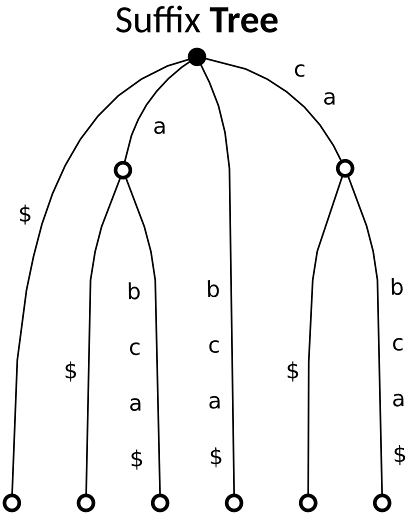
- Special **sentinel character** \$ not part of Σ
- Consider the suffix tree of $s\$$ (instead of s)
- Implies bijection between suffixes and leaves

Example: Constructing a Suffix Tree

`cabca$`

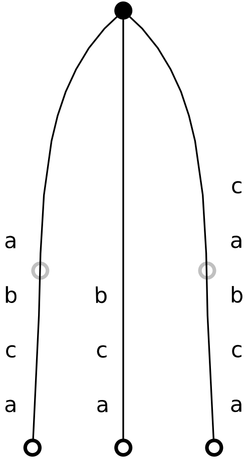
Suffix Trie vs. Suffix Tree





Implicit vs. Explicit Suffix Tree

T=cabca

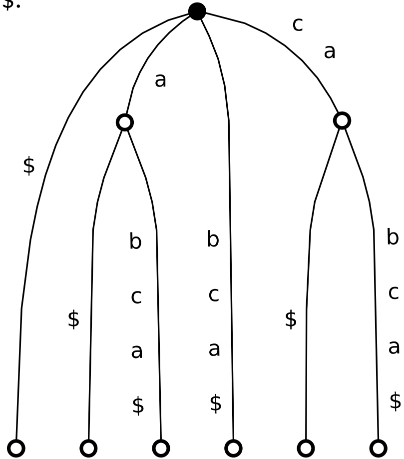


implicit suffix tree

suffixes of T$:

0	cabca$
1	abca$
2	bca$
3	ca$
4	a$
5	$

T$=cabca$



Using Suffix Trees for Pattern Matching

Flavors of pattern searching

1. **Decision:** Is P a substring of s?
2. **Counting:** How often does P occur in s?
3. **Enumeration:** At what positions does P occur in s?

Black board: Suffix Trees for Pattern Matching

Runtimes: Using Suffix Trees for Pattern Matching

Flavors of pattern searching

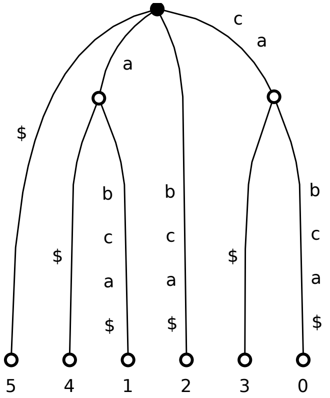
1. **Decision:** Is P a substring of s?
   $\rightarrow O(m)$
2. **Counting:** How often does P occur in s?
   $\rightarrow O(m + k)$
3. **Enumeration:** At what positions does P occur in s?
   $\rightarrow O(m + k)$

Note: $m = |P|$ and k is the number of occurrences.

Applications: Longest repeated substring

Given $s \in \Sigma^*$. The suffix tree of $s\$$ spells all substrings of $s\$$.

- **Question:** how do you find the longest repeated substring?

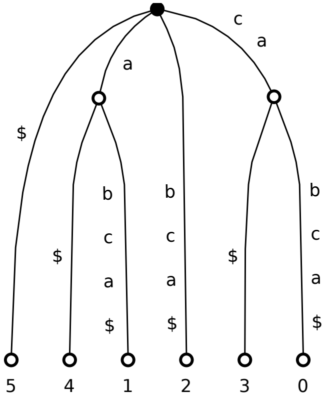


Suffix tree for $s = cabca\$$

Applications: Longest repeated substring

Given $s \in \Sigma^*$. The suffix tree of $s\$$ spells all substrings of $s\$$.

- **Question:** how do you find the longest repeated substring?
- **Answer:** A substring t of s occurs more than once if after reading t from the root you end in an **inner node** or on an edge above an inner node. So the longest repeated substring can be found as the inner node with the longest path label (largest string depth) in a tree traversal.



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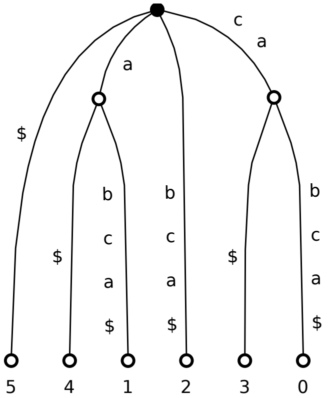
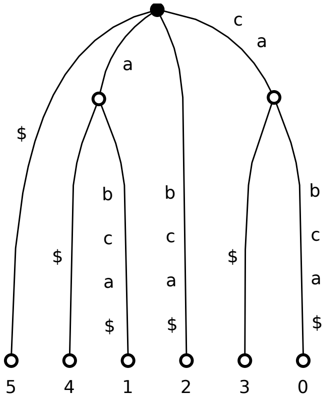


Suffix tree for $s = cabca\$$

Applications: Shortest unique substring

- **Question:** how do you find the shortest unique substring (without the sentinel)?
- **Answer:** Unique substrings end in a leaf edge in the tree. We look for the **inner node** v (including the root node) with the **shortest path label** that does **contain a leaf edge** that is not simply the $ character. Path label v plus the first letter on the leaf edge denotes the shortest unique substring.



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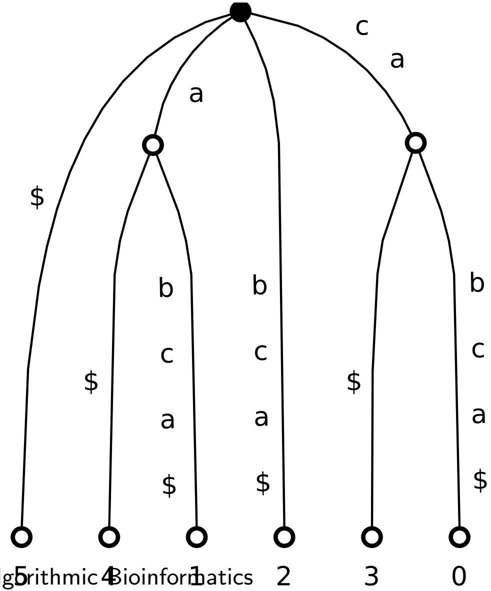
Linear Time Suffix Tree Construction

Issues to be solved



Naive implementation

- Space consumption?
- Construction time?

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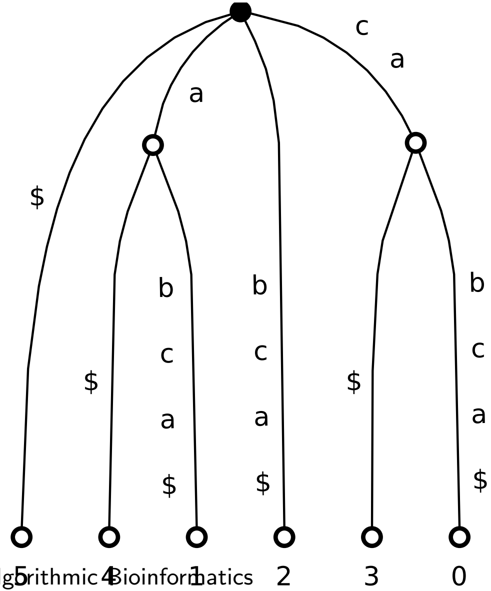

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  $O(n^2)$
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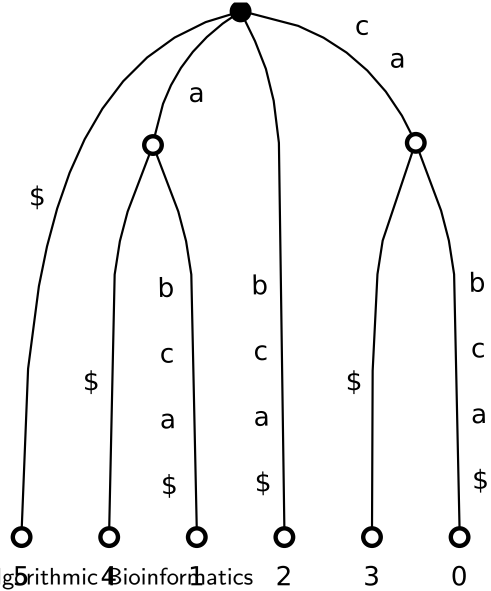

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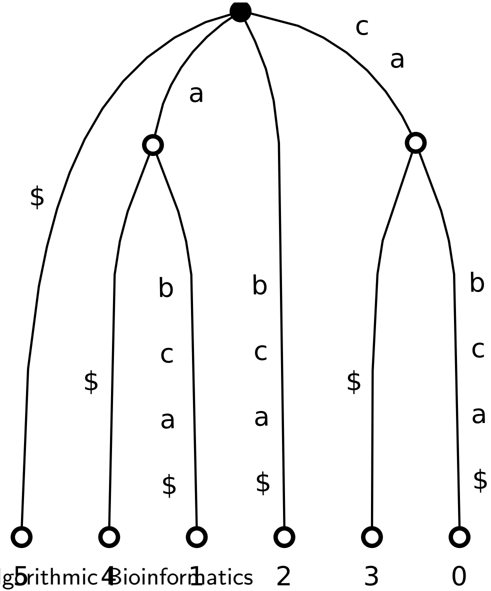

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  $O(n^2)$
- Construction time?
  $O(n^2)$

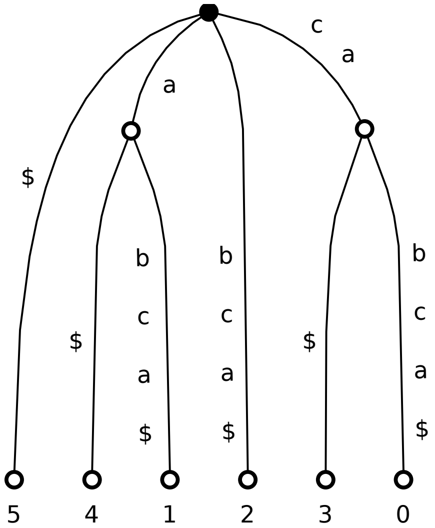
Goals

- Linear space: $O(n)$
- Linear time: $O(n)$

History of linear time suffix tree algorithms

- Peter Weiner introduced suffix trees in 1973
  (named bi-tree at the time, algorithm of the year)
- Edward McCreight 1976 (starting from longest suffixes)
- Esko Ukkonen introduced an on-line algorithm in 1992,
  later known as Ukkonen's algorithm (we will do this one)

Number of Nodes and Edges



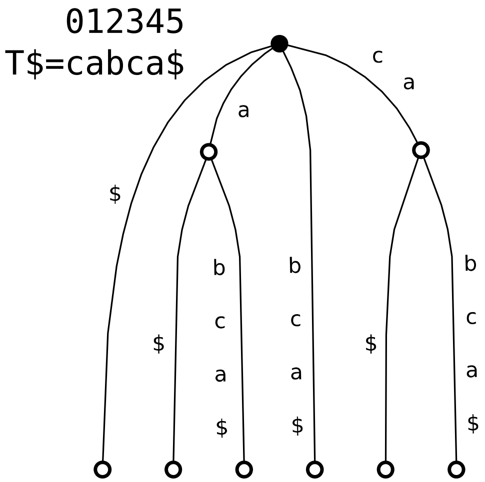
Lemma

A suffix tree of string $T\$$ with $|T\$| = n$ has exactly n leaves. There exist at most $n-1$ inner nodes and at most $2(n-1)$ edges.

Proof

Try at home...

Space Consumption



Space

- Edge labels take $O(n^2)$ space

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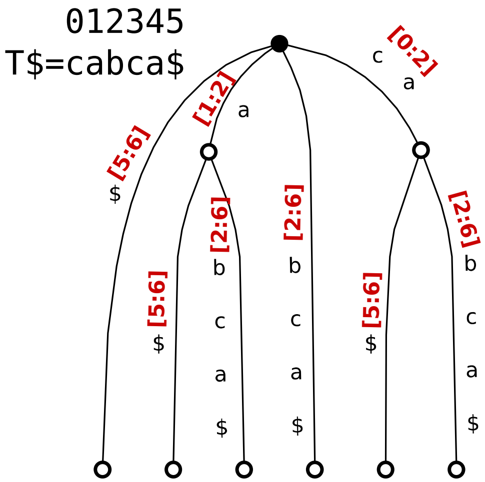


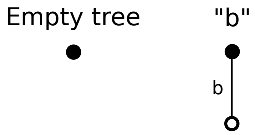
Space

- Edge labels take $O(n^2)$ space
- **Indices** into T take $O(1)$ per edge, and $O(n)$ in total

Idea: Online Construction (babacacb$)

Empty tree

Idea: Online Construction (babacacb$)



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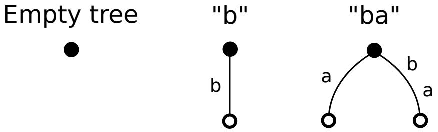

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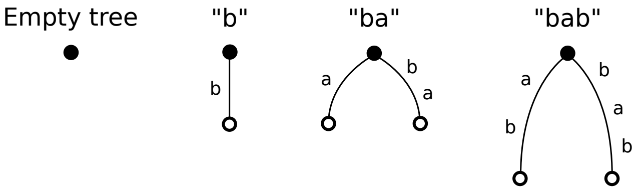

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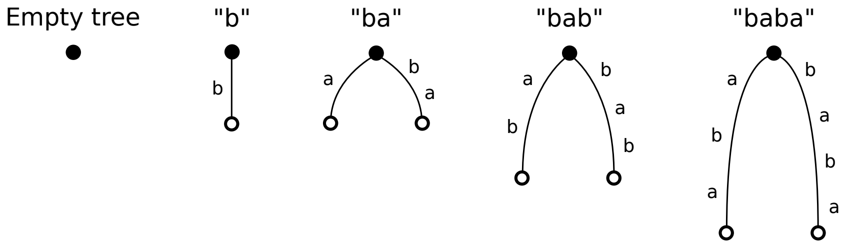

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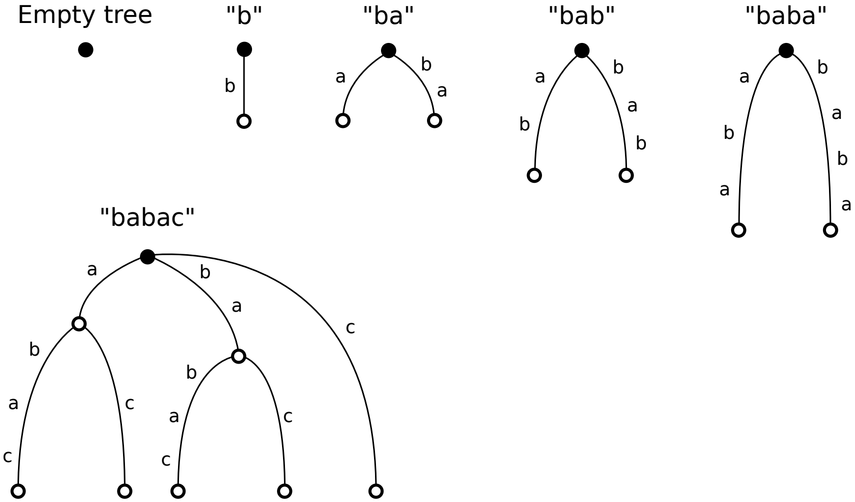

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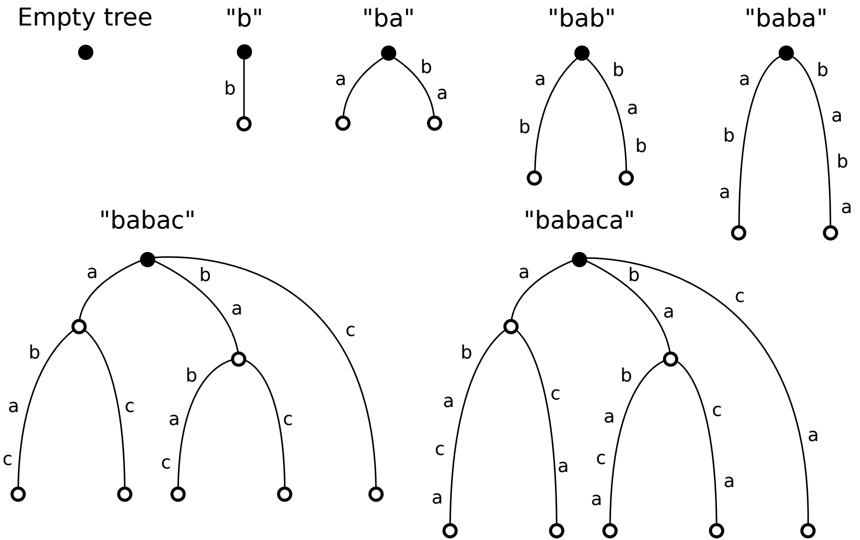


Online Construction

Key Question

How can we achieve linear time when we extend $O(n)$ different suffixes in each step?

Example:

- Suffix tree of `bab` contains suffixes `bab`, `ab`, `b`.
- Suffix tree of `baba` contains suffixes `baba`, `aba`, `ba`, `a`.

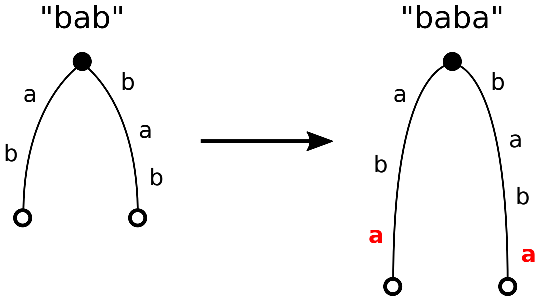
Ukkonen's algorithm

- Rule I: implicit leaf extension
- Rule II: new leaf creation
- Rule III: already represented

Rule I: Implicit Leaf Extension

Scenario

Suffix ends in a leaf.



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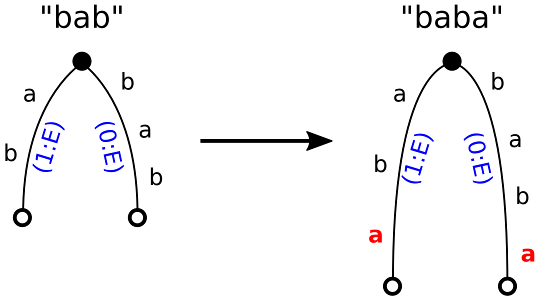


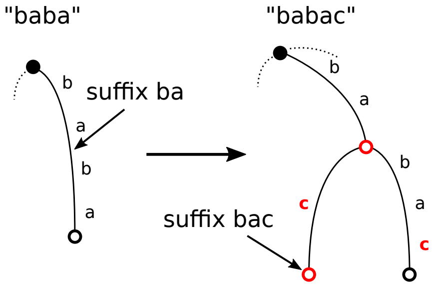
Approach

Special end marker “E”: substring up to the end of the current text

Rule II: New Leaf Creation

Scenario

Suffix ends inside tree (edge label or at inner node),
new **character not yet present** below this position in the tree



Approach

Insert leaf. Create inner node if suffix ends inside edge label.

Rule III: Already Represented

Scenario

Suffix ends inside tree (edge label or at inner node),
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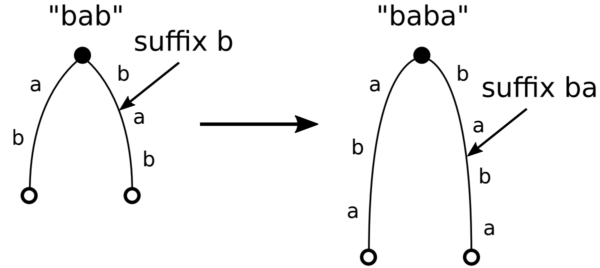

Approach

No need to do anything.

Rule Example

	suffix starting at					
	0	1	2	3	4	5
Phase 0	2					
Phase 1						
Phase 2						
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Phase 4						
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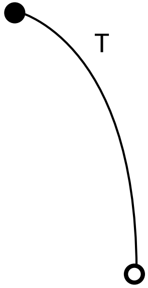
TAATA$
012356



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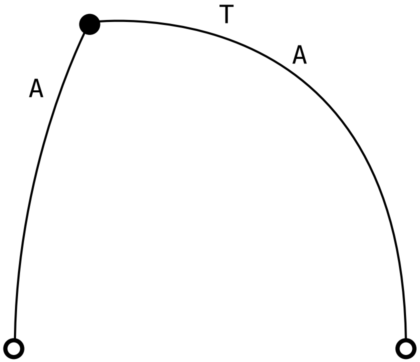

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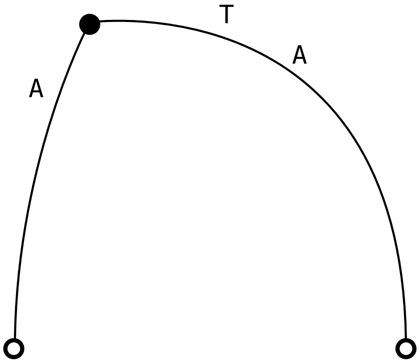

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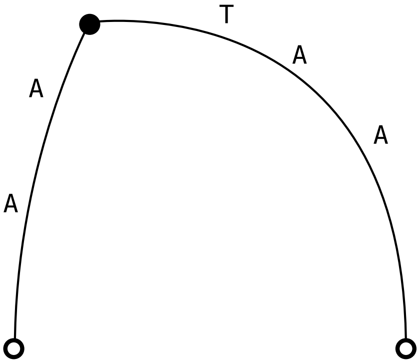

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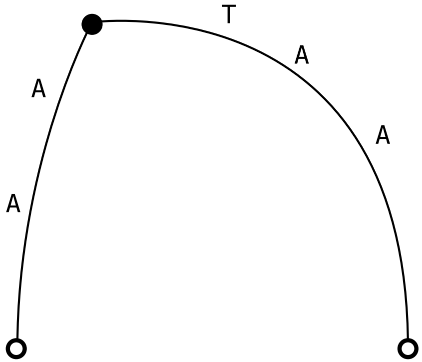

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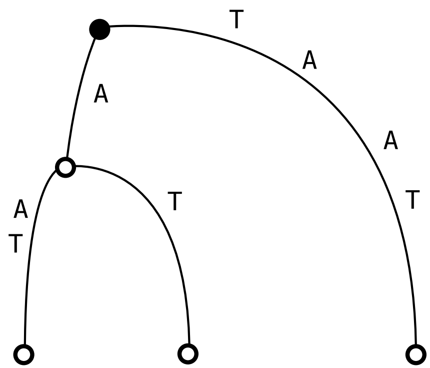

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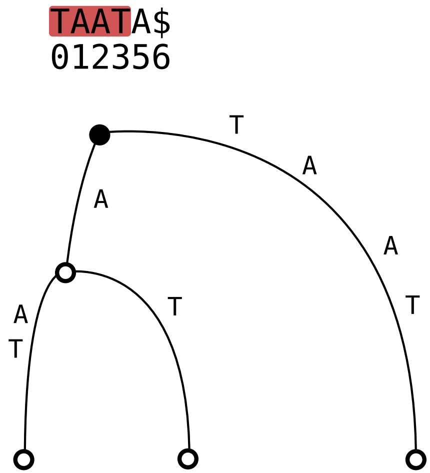

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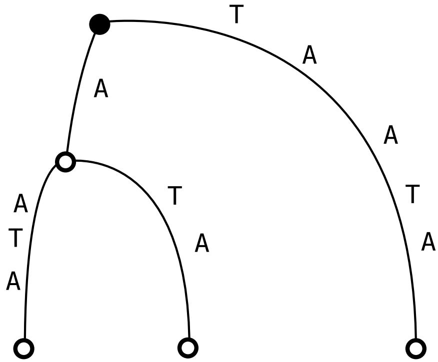

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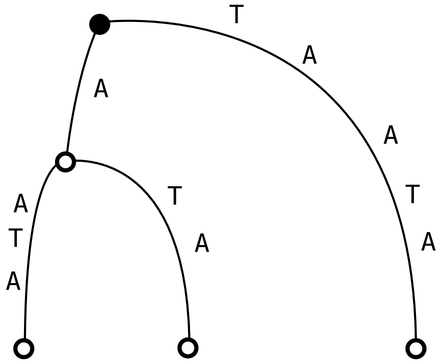

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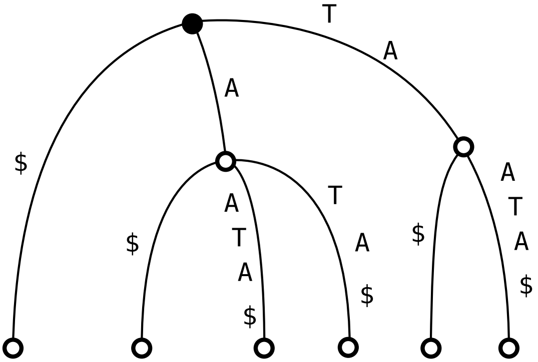

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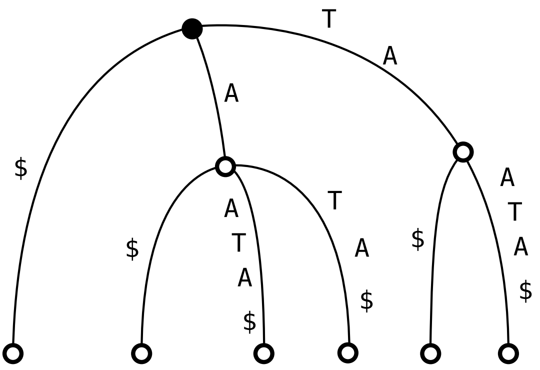


Ukkonen's Algorithm: Open Questions

Situation

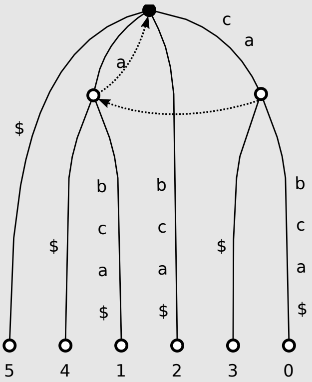
- We need to apply Rule 2 exactly n times:
  Rule 2 for the suffix starting at i is used in one phase $\geq i$.
- Rule 1 does not entail any work to be done (zero time!)
- Rule 3 only moves the active position down by one character ($O(1)$ time)

Missing ingredients

- How do we know when to apply which rule?
- How do we locate positions in the tree that require work?
- How do we implement Rule II to run in constant time?

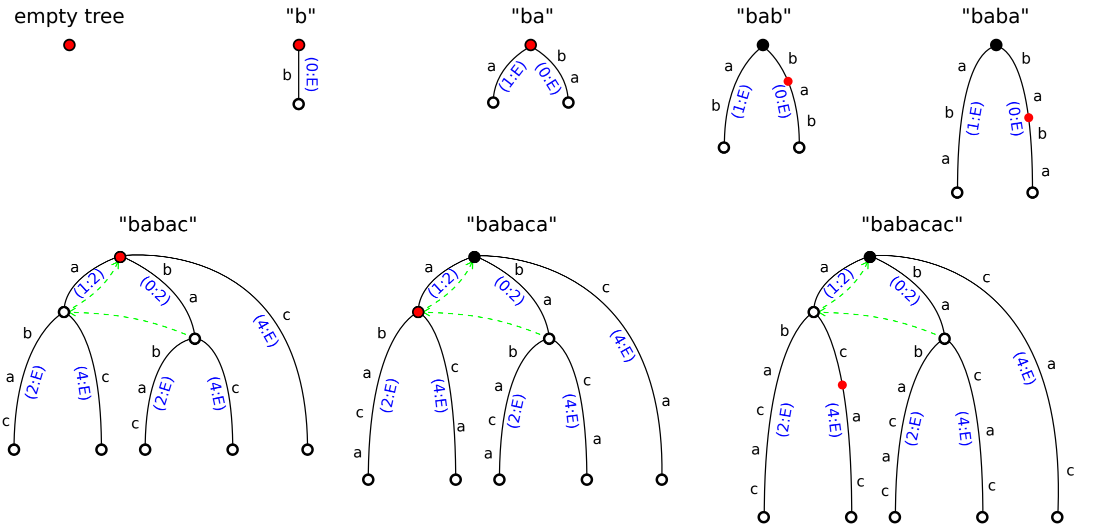
Suffix links

Suffix tree for $T = \texttt{cabca\$}$:



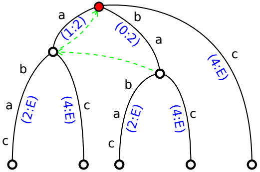
For an internal node v with path label $c\alpha$, $c \in \Sigma$, $\alpha \in \Sigma^*$, there is another node v', with path label α (why?).
An edge $v \to v'$ (string $c\alpha \to \alpha$) is a **suffix link** ("cut off the first character").

Ukkonen Example (babacacb$)

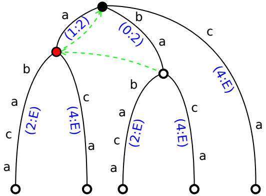


Ukkonen Example (babacacb$)

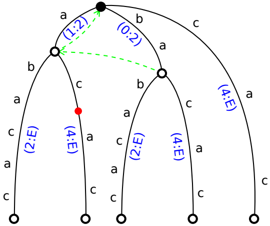
"babac"



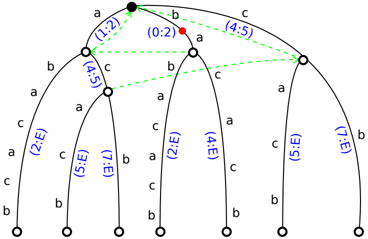
"babaca"



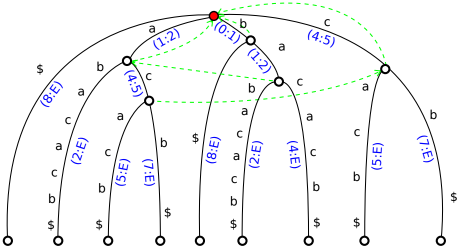
"babacac"



"babacacb"



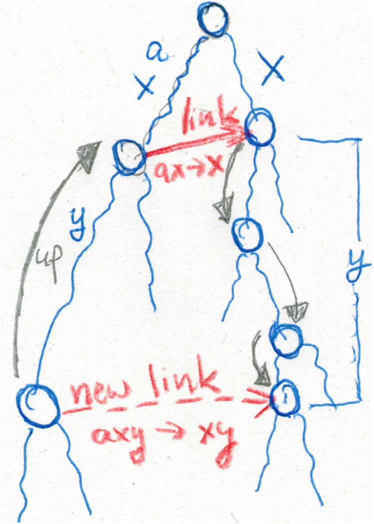
"babacacb$"



Suffix Links: Skip & Count

Skip & Count Trick

1. From active position (node axy), jump up to parent node ax, count $|y|$ in $O(1)$ time.
2. Use suffix link to x in $O(1)$ time
3. Walk down along y, hop from node to node, skipping & counting characters in $O(h_i)$ time, with h_i: number of hops for phase i.



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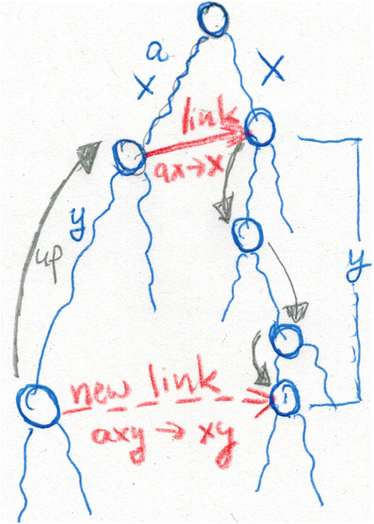
- Need to show in fact $\sum_{i=0}^{n-1} h_i = O(n)$:



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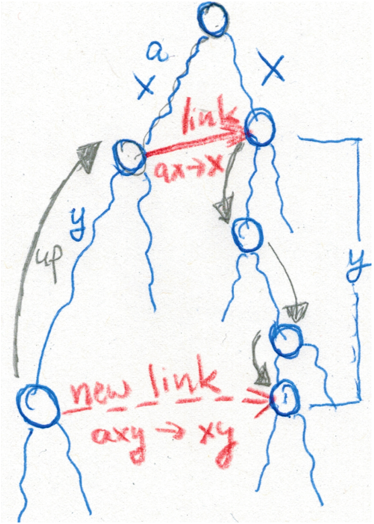
- Node depth cannot increase arbitrarily: $\leq n$.
- Each leaf insertion decreases depth by ≤ 1.



Ukkonen's Suffix Tree Construction

Text $T\$$ with $n = |T\$|$: Construction uses n phases $i = 0, \dots, n-1$.

Initialization

- Start with a root-only tree. The **active position** is the root.

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Phase i with $j \leq i$ leaves already inserted

1. Apply Rule 1 for each existing leaf (implicit leaf extension); no time
2. Check whether $T[i]$ already exists from the active position:
   If yes, apply Rule 3, move active position down, done.
3. If not, start inserting leaves $j, j+1, \dots$ up to i or until Rule 3 applies.
   To move from j to $j+1$, use existing suffix links and insert new suffix links.

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Termination

- $T[n-1] = \$$ is unique. All missing leaves are automatically created.
- Finally, replace end marker E by $n-1$ on each edge.

Implementation Notes

Active position

The active position can be represented as a triple (v, c, ℓ),
with a node v, character c of an outgoing edge,
and number of characters $\ell \geq 0$ along that edge.

Data structures for children of a node

Consider a node with c children, $c \leq |\Sigma|$:

	space/node	access time	total space	used for
linked list	$O(c)$	$O(c)$	$O(n)$	large alphabets
array	$O(\|\Sigma\|)$	$O(1)$	$O(n\|\Sigma\|)$	small alphabets
balanced tree	$O(c)$	$O(\log c)$	$O(n)$	large alphabets
hash table	$O(c)$	$O(1)$	$O(n)$	very large alphabets

Summary

Today

- **Suffix trees**
- **Applications**
  - Pattern matching
  - Longest repeated substring
  - Shortest unique substring
- Ukkonen's algorithm: linear time **suffix tree** construction
  - substring representation on edges by indices
  - implicit zero-time edge extension by end marker E
  - suffix links
  - skip & count trick: amortized analysis
- **Suffix links:** useful also in other contexts

Exam Questions

- Define a suffix tree. What is a suffix trie?
- Construct the suffix tree with suffix links of an example string.
- What is the running time of pattern search with a suffix tree?
- How can the longest repeated substring problem and the shortest unique substring problem be solved in optimal time with suffix trees?
- Explain Ukkonen's algorithm.
- What is the important trick to achieve linear space consumption in Ukkonen's algorithm?
- What is a suffix link? What are suffix links used for in Ukkonen's algorithm?
- Apply Ukkonnen's algorithm to an example string.
- Why does Ukkonen's algorithm run in $O(n)$ time?
- Explain the skip & count trick.
- Explain how one could implement the elements of a suffix tree.
  What are alternative ways of storing the children of a suffix tree node?