Efficient Index for Weighted Sequences

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Weighted Sequences

Weighted sequence (position weight matrix, PWM):
probability of occurrence $\pi_i(a)$ for each position i and letter $a \in \Sigma$.

$$\sum_{a \in \Sigma} \pi_i(a) = 1$$

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
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Encodes probability distribution on solid strings:

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Match specified by **threshold** (cut-off) probability $\frac{1}{z}$.

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Encodes probability distribution on solid strings:

$\frac{1}{z} = \frac{1}{8}$ b a b a a probability $\frac{3}{32} < \frac{1}{8}$ NO

Match specified by **threshold** (cut-off) probability $\frac{1}{z}$.

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Weighted Sequences: Motivation

Origin

Computational biology:

1982 Stormo, Schneider, Gold, and Ehrenfeucht
Nucleic Acids Research.

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Primary use

Motifs in biological sequences.

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Related notion

Profiles (scoring matrices):

- additive (as $\log \pi_i(a)$),
- arbitrary scores (no equivalent of $\sum_{a \in \Sigma} \pi_i(a) = 1$ constraint).

Problems Studied

Pattern matching and indexing

Christodoulakis et al., 2004
Iliopoulos et al., 2006
Amir et al., 2008

Approximate and gapped pattern matching

Zhang et al., 2004
Amir et al., 2006
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Repetitions and regularities discovery

Iliopoulos et al., 2005
Christodoulakis et al., 2006
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Barton and Pissis, 2014

Longest common subsequence problem

Amir et al., 2009
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Alignment of weighted sequences

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Indexing for Weighted Pattern Matching

Input

T – weighted sequence of length n over alphabet of size σ

($\sigma = \mathcal{O}(1)$ in this talk)

$\frac{1}{z}$ – threshold probability

Query Input

P – string pattern of length m

Query Output

$\mathrm{Occ} = \{i : P \text{ matches } T[i, i+m-1] \text{ with probability } \geq \frac{1}{z}\}$

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$\frac{1}{z} = \frac{1}{8}$ $\quad P = \mathtt{aba}$

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a b a

$\frac{1}{z} = \frac{1}{8}$ $P = \mathtt{aba}$ probability $0 < \frac{1}{8}$ NO $\mathrm{Occ} = \{\}$

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a b a

$\frac{1}{z} = \frac{1}{8}$ $P = \mathtt{aba}$ probability $\frac{1}{8} \geq \frac{1}{8}$ YES $\mathrm{Occ} = \{2\}$

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a b a

$\frac{1}{z} = \frac{1}{8}$ $P = \mathtt{aba}$ probability $\frac{3}{8} \geq \frac{1}{8}$ YES $\mathrm{Occ} = \{2, 3\}$

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$\frac{1}{z} = \frac{1}{8}$ $\quad P = \mathtt{aba}$ $\quad \mathrm{Occ} = \{2, 3\}$

Results

Iliopoulos et al., 2006:

- $\mathcal{O}(n \cdot f(z))$ space
- $\mathcal{O}(n \cdot f(z))$ construction time
- $\mathcal{O}(m + |\mathrm{Occ}|)$ query time

Amir et al., 2008:

- $\mathcal{O}(nz^2 \log z)$ space
- $\mathcal{O}(nz^2 \log z(\log\log z + \log\log n))$ construction time
- $\mathcal{O}(nz^2 \log z)$ construction time follows from later results: Iliopoulos & Rahman, 2008; Juan et al. 2009
- $\mathcal{O}(m + |\mathrm{Occ}|)$ query time

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Our results:

- $\mathcal{O}(nz)$ space
- $\mathcal{O}(nz)$ construction time
- $\mathcal{O}(m + |\mathrm{Occ}|)$ query time

Maximal solid factors

Solid factor: an occurrence of a string (at a particular position)

Maximal solid factor: cannot be extended to an occurrence of a superstring

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Probability: $\frac{1}{4} \geq \frac{1}{8}$

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Probability: $\frac{3}{16} \geq \frac{1}{8}$

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Probability: $\frac{1}{8} \geq \frac{1}{8}$

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Naive solution: Pattern matching in all maximal solid factors.

- Might be of length $\Theta(n^2 z)$ in total.

Previous approach

Heavy character: highest probability at the given position.

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b	a	b		
	a	b	a	a
	a	b	b	a

Amir et al. (reinterpreted):

1. Merge overlapping solid factors with equal heavy extensions.

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2. Each position covered by $\mathcal{O}(z^2 \log z)$ factors.

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	a	b	a	a

Amir et al. (reinterpreted):

1. Merge overlapping solid factors with equal heavy extensions.
2. Each position covered by $\mathcal{O}(z^2 \log z)$ factors.
3. **Property matching** in the resulting factors:
   upper bound on fragment length for each starting position.

Our approach

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
b $\frac{3}{4}$	b 0	b $\frac{1}{4}$	b $\frac{1}{2}$	b 0

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b	a	a	a	a
b	a	a	b	a
b	a	b		
	a	b	a	a
	a	b	b	a

Our approach:

Our approach

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
b $\frac{3}{4}$	b 0	b $\frac{1}{4}$	b $\frac{1}{2}$	b 0

a	a	a	b	a
b	a	a	a	a
b	a	a	b	a
b	a	b	b	a
	a	b	a	a
	a	b	b	a

Our approach:

1. Extend each maximal solid factor to the right.

Our approach

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
b $\frac{3}{4}$	b 0	b $\frac{1}{4}$	b $\frac{1}{2}$	b 0

a	a	a	b	a
b	a	a	a	a
b	a	a	b	a
b	a	b	b	a
	a	b	a	a
	a	b	b	a

Our approach:

1. Extend each maximal solid factor to the right.
2. Build a trie of (the reverses of) the obtained suffixes.

Our approach

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
b $\frac{3}{4}$	b 0	b $\frac{1}{4}$	b $\frac{1}{2}$	b 0

b	a	a	b	a
a	a	a	b	a
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a				
b	a	b		
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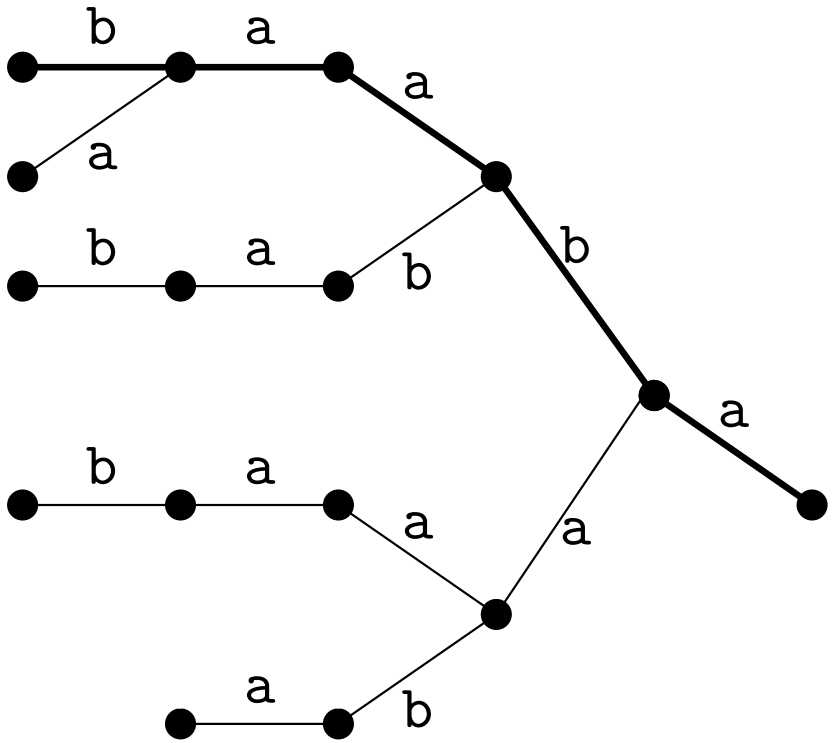
Our approach:

1. Extend each maximal solid factor to the right.
2. Build a trie of (the reverses of) the obtained suffixes.
3. Property matching in a trie of $\mathcal{O}(nz)$ nodes.

Trie size

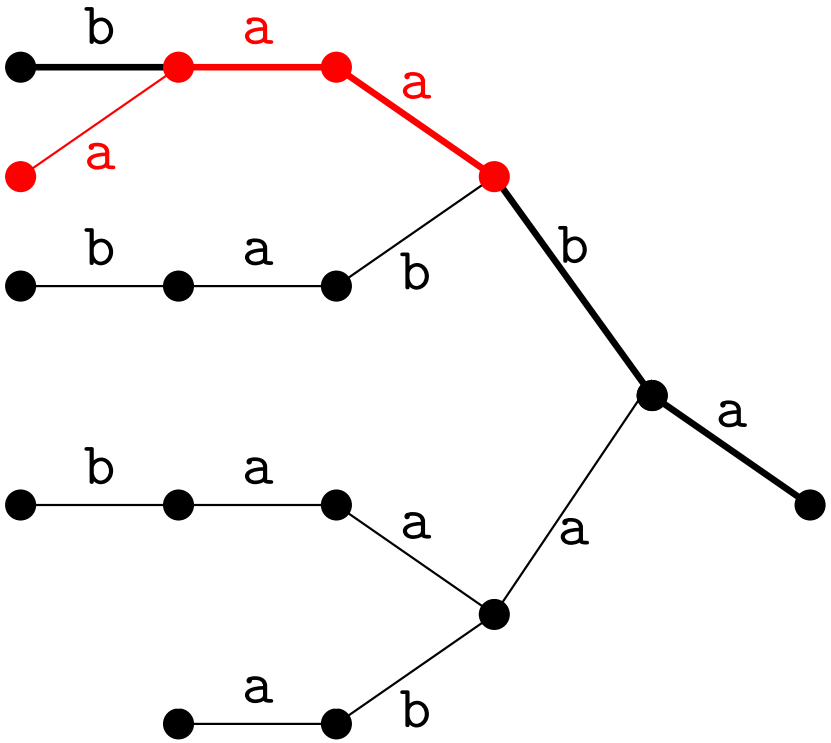
a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
b $\frac{3}{4}$	b 0	b $\frac{1}{4}$	b $\frac{1}{2}$	b 0



Bijection: nodes $\leftrightarrow$ right-maximal solid factors.

Trie size

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
b $\frac{3}{4}$	b 0	b $\frac{1}{4}$	b $\frac{1}{2}$	b 0



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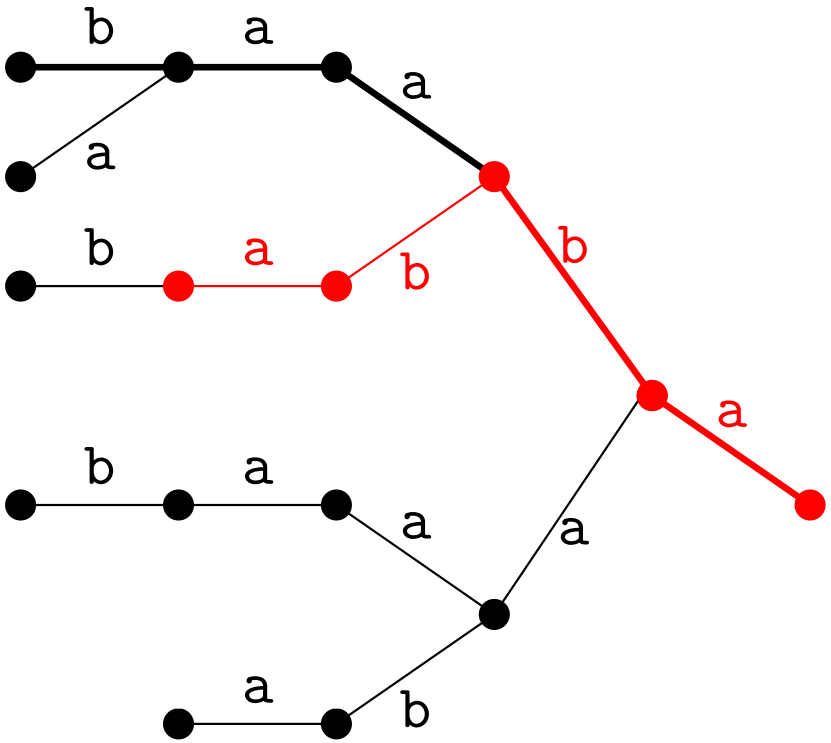

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Trie size

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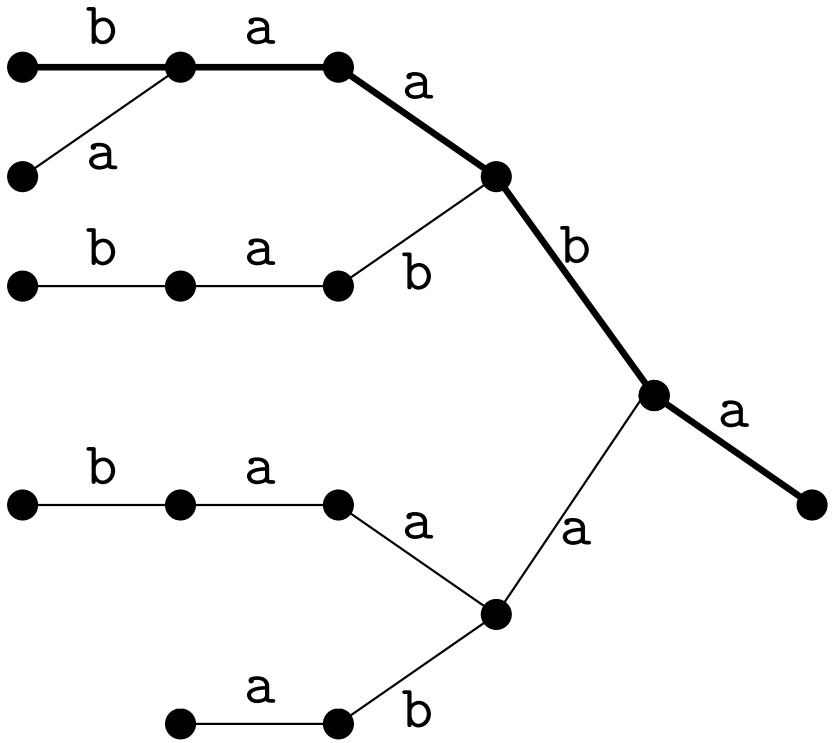

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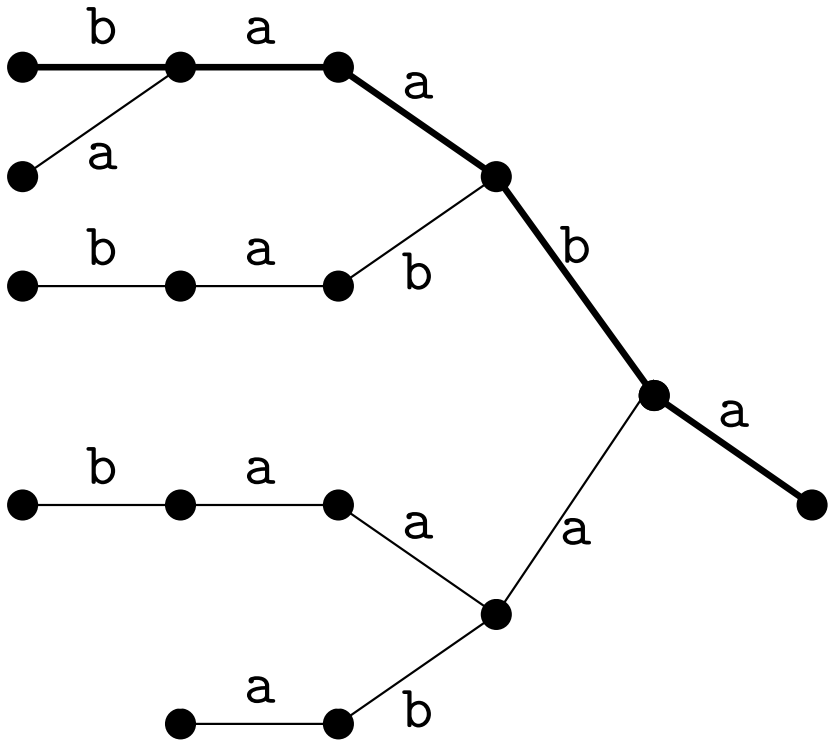

Bijection: nodes $\leftrightarrow$ right-maximal solid factors.

Fact [Amir et al.]: $\leq z$ right-maximal solid factors start at any i.

Trie construction

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
b $\frac{3}{4}$	b 0	b $\frac{1}{4}$	b $\frac{1}{2}$	b 0

Level-by-level **construction**: for each node:

Trie construction

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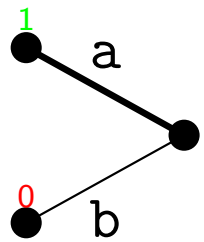

Trie construction

a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
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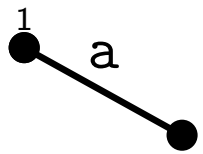
Level-by-level **construction**: for each node:

1. extend to the left using every possible character,
2. trim leaves with prob. $< \frac{1}{z}$ counting from the heavy path.



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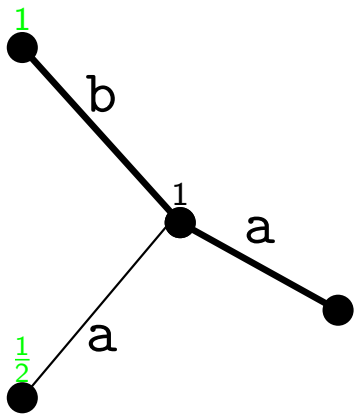

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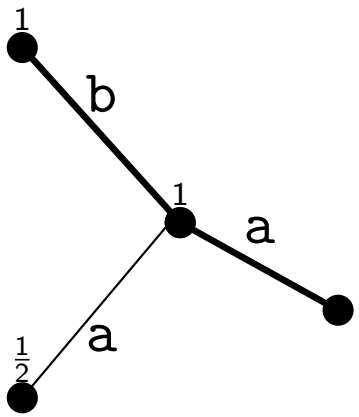

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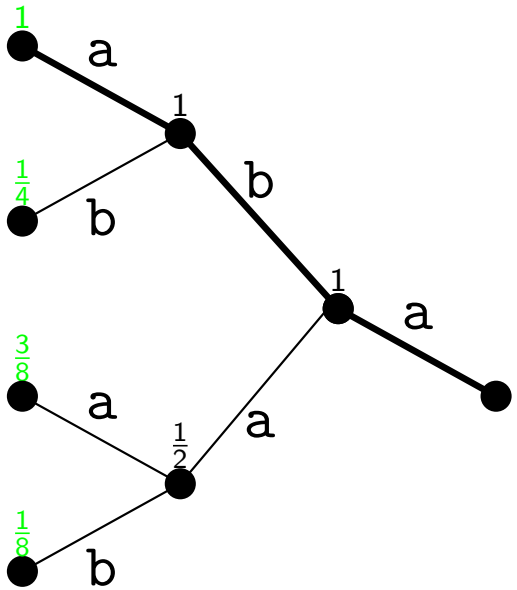

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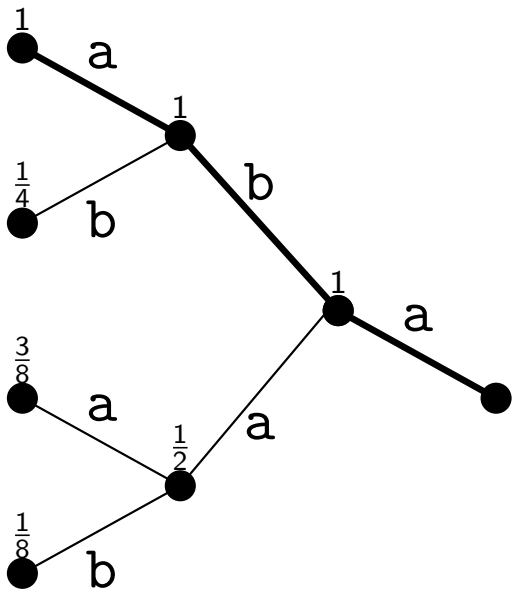

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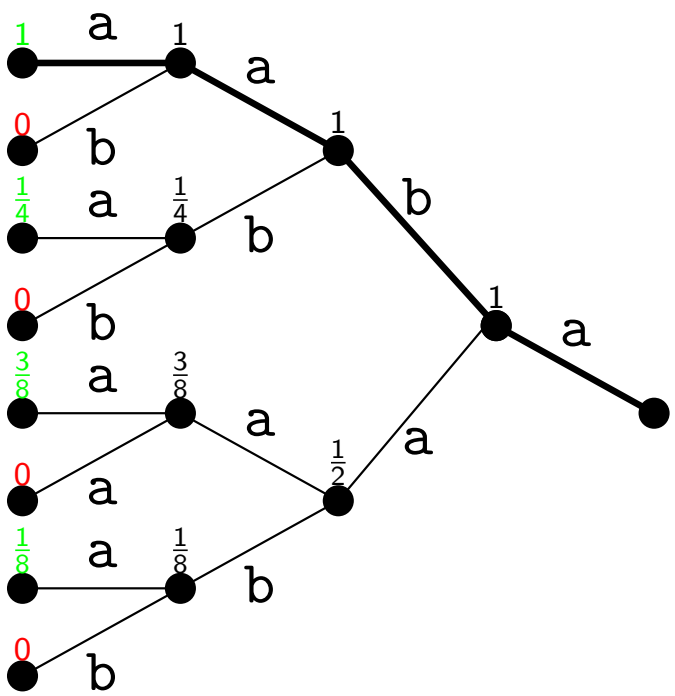

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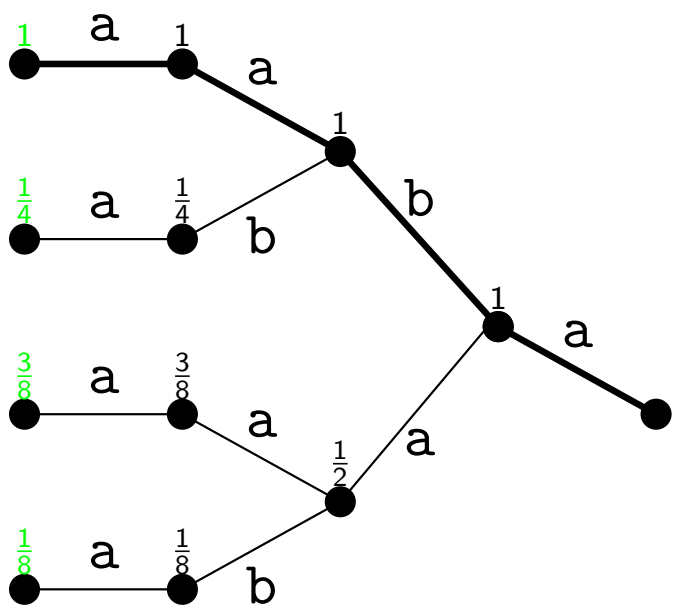

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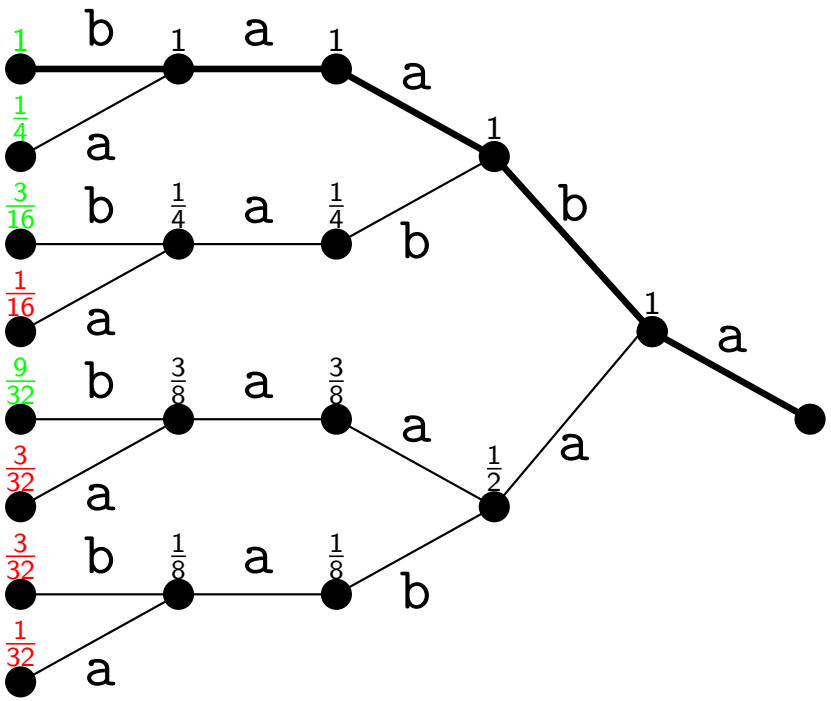

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a $\frac{1}{4}$	a 1	a $\frac{3}{4}$	a $\frac{1}{2}$	a 1
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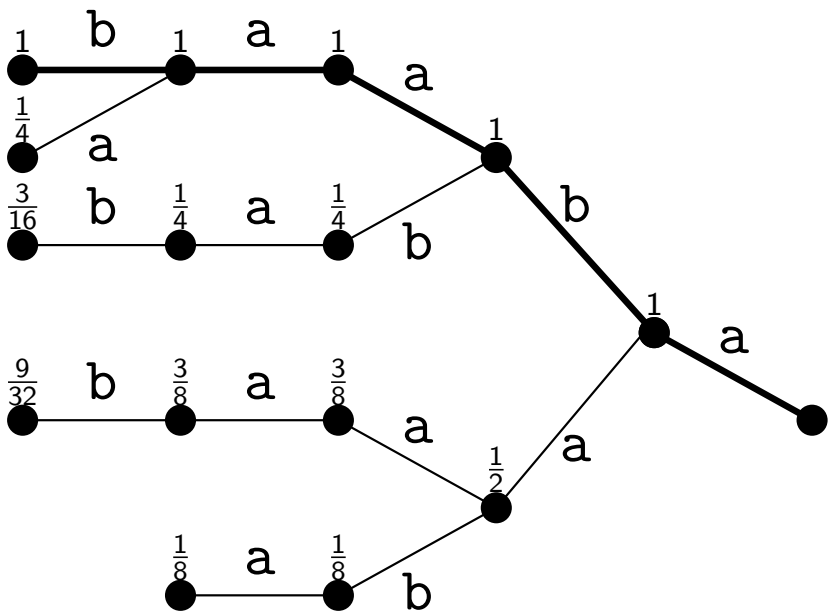

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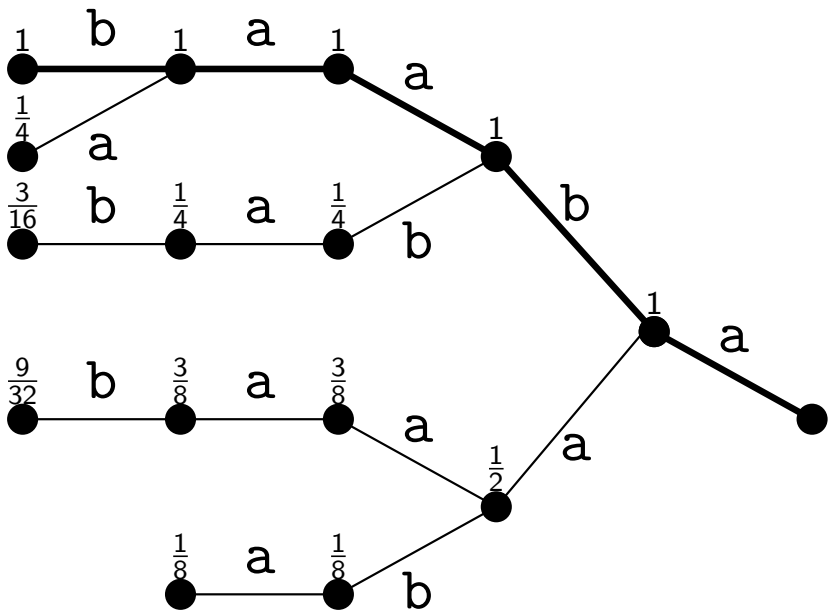

Upper bounds for property matching:
generate the bijection via a left-to-right traversal.

Weighted index construction

Suffix tree of a trie:
Compressed trie of paths from each node of the trie to the root.

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Suffix tree (of a trie) $\rightarrow$ property suffix tree (of a trie)
Each terminal node needs to be moved up.
Many solutions, e.g.:

1. Use off-line weighted level ancestors
   - linear-time using the special case of union-find.
2. Trim everything without a new terminal node in the subtree.

Answering queries

Queries for a pattern P of length m.

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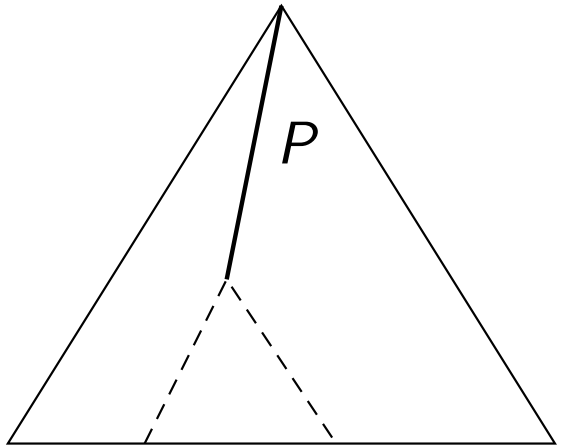
Decision version: $\mathcal{O}(m)$ time

- traverse the suffix tree with P.

Property suffix tree:



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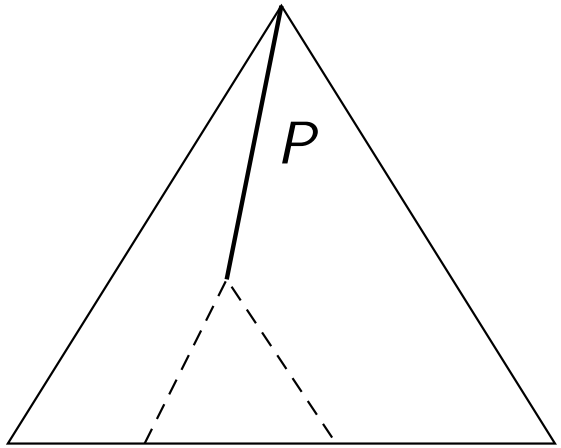

Reporting: $\mathcal{O}(m + |\mathrm{Occ}|)$ time

- report all terminal nodes in the subtree?

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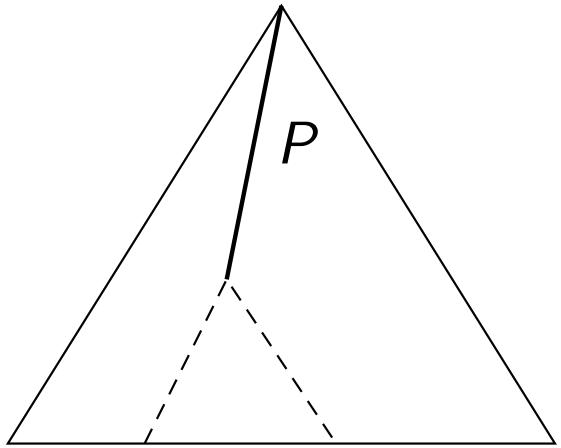

Reporting: $\mathcal{O}(m + |\mathrm{Occ}|)$ time

- report all terminal nodes in the subtree? Repeating occs.

Answering queries

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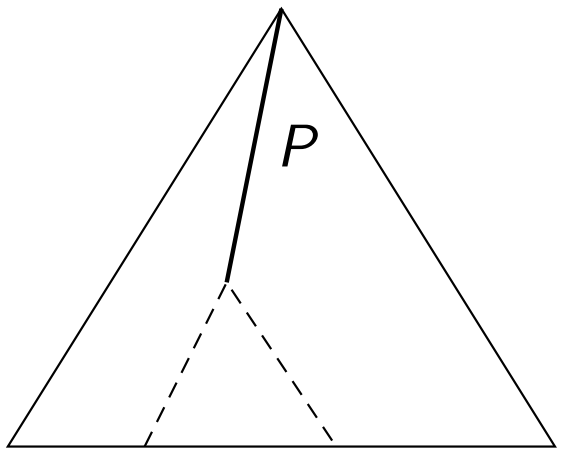

Queries for a pattern P of length m.

Decision version: $\mathcal{O}(m)$ time

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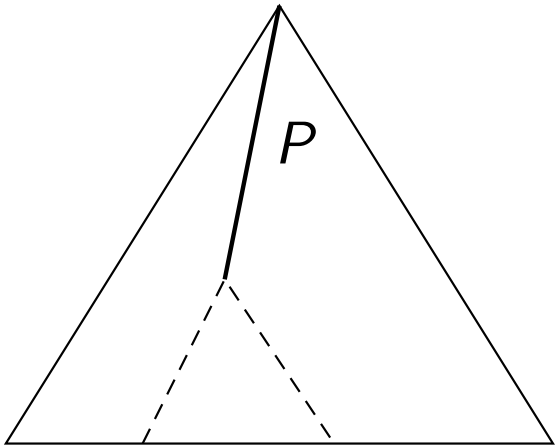

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Lemma [Muthukrishnan] Colored range listing:
Report distinct elements in a given range of a preprocessed array.

Answering queries

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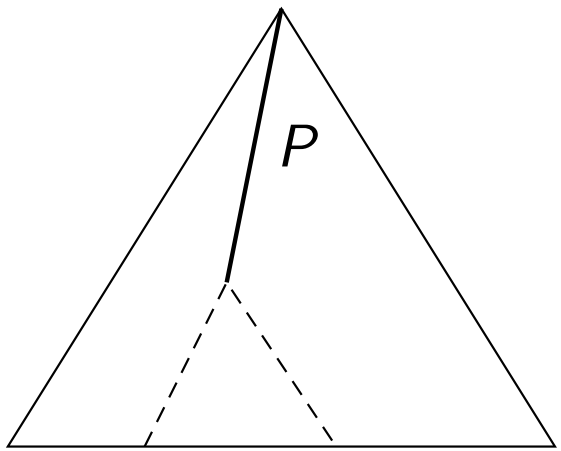

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Answering queries

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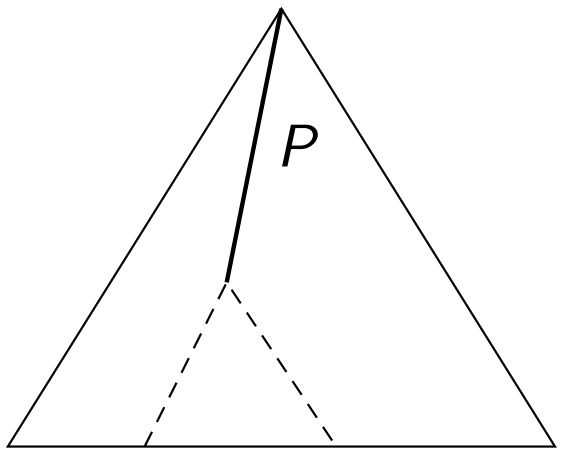

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Lemma [Hui] Colored set size:
Count the number of distinct leaf colors for each node (offline).

Applications

Longest common extension:

$\mathrm{LCE}(i, j) =$ length of the longest solid factor occurring in i and j

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Example: For $\frac{1}{z} = \frac{1}{8}$, $\mathrm{LCE}(1, 2) = 3$ (aaa).

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Covers: $\mathcal{O}(nz)$ time
solid strings whose occurrences cover all positions of the text.

Summary and open problems

Index for weighted pattern matching:

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- $\mathcal{O}(nz)$ construction time,
- $\mathcal{O}(m + |\mathrm{Occ}|)$ query time (reporting),
- $\mathcal{O}(m)$ query time (counting).

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Open problems:

- support queries with $z' < z$,
  - Biswas et al. (EDBT'16) achieve this for $z = \mathcal{O}(1)$.
- support weighted patterns in $o(z(m + |\mathrm{Occ}|))$ time.

Questions?

Thank you for your attention!