Suffix Trees

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Algorithms on Strings
Data Structures and Algorithms

This slide desk is incomplete.
For the complete set of frames,
please see our videos in the
Algorithms on Strings course on Coursera
(Algorithms and Data Structures Specialization)

Outline

- **From Genome Sequencing to Pattern Matching**
- Brute Force Approach to Pattern Matching
- Herding Patterns into Trie
- Herding Text into Suffix Trie
- From Suffix Tries to Suffix Trees

The Newspaper Problem

stack of NY Times, June 27, 2000

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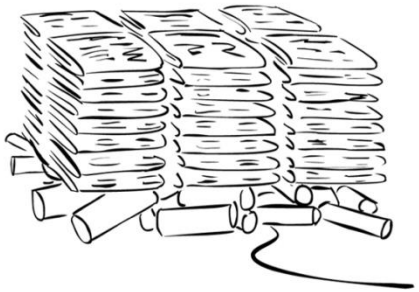
stack of NY Times, June 27, 2000



stack of NY Times, June 27, 2000
on a pile of dynamite

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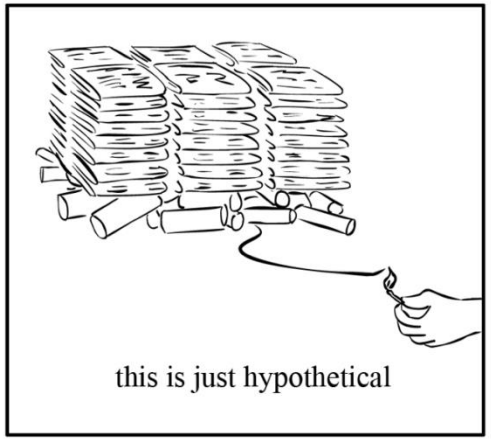

this is just hypothetical

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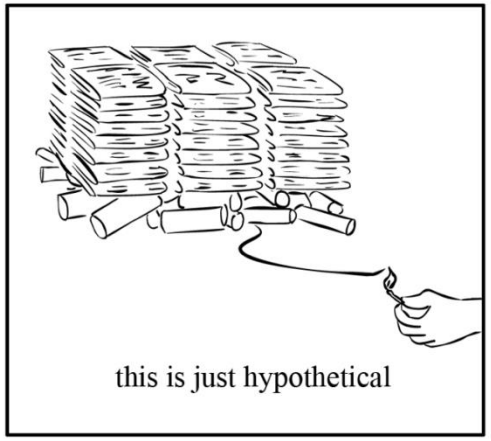

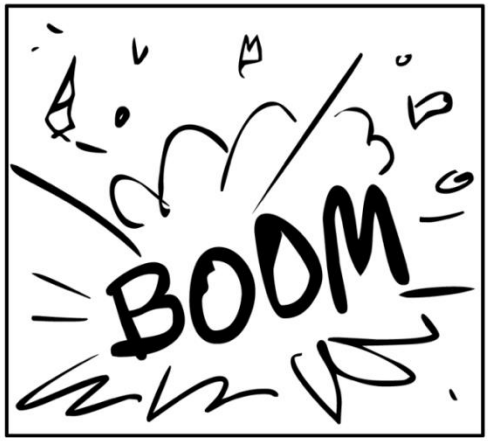

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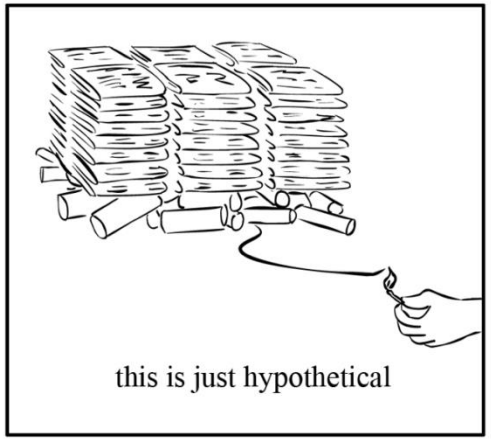

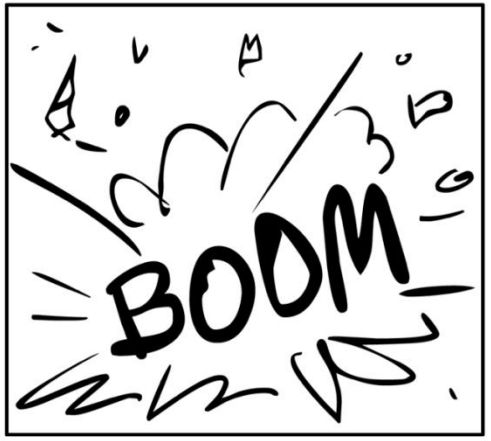

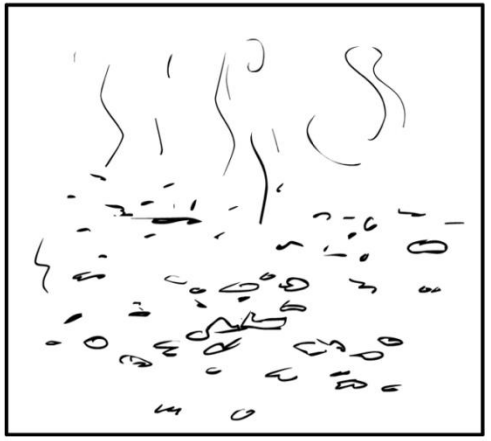

The Newspaper Problem

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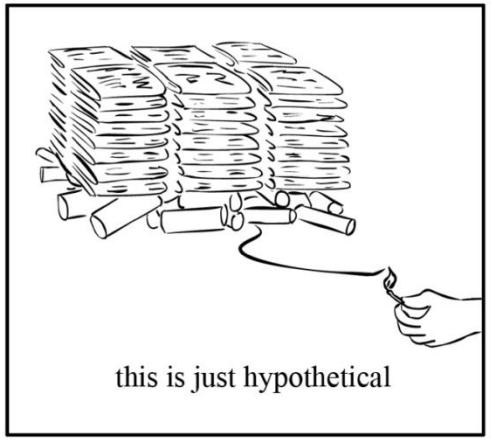

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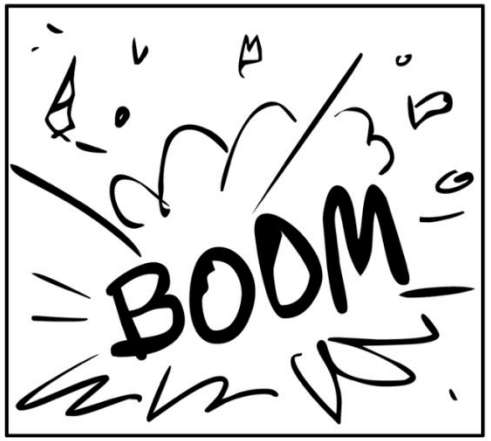
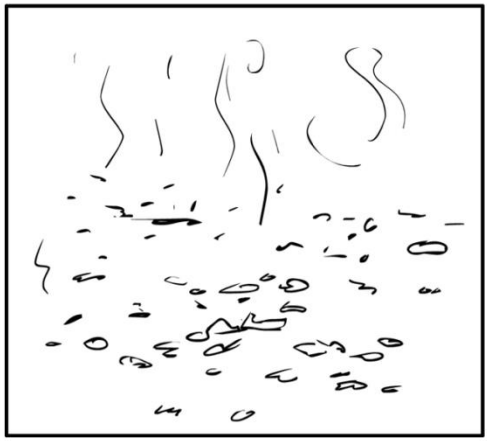
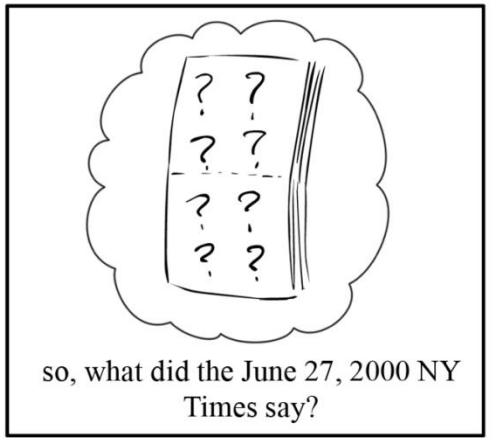
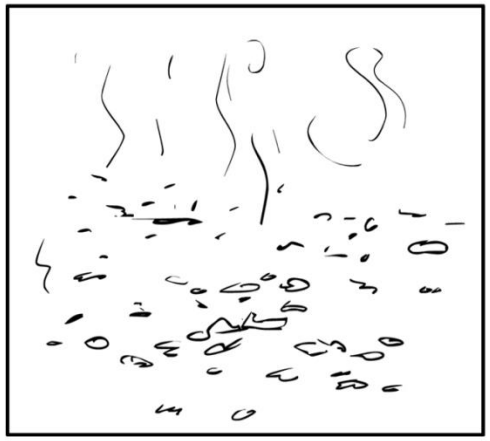


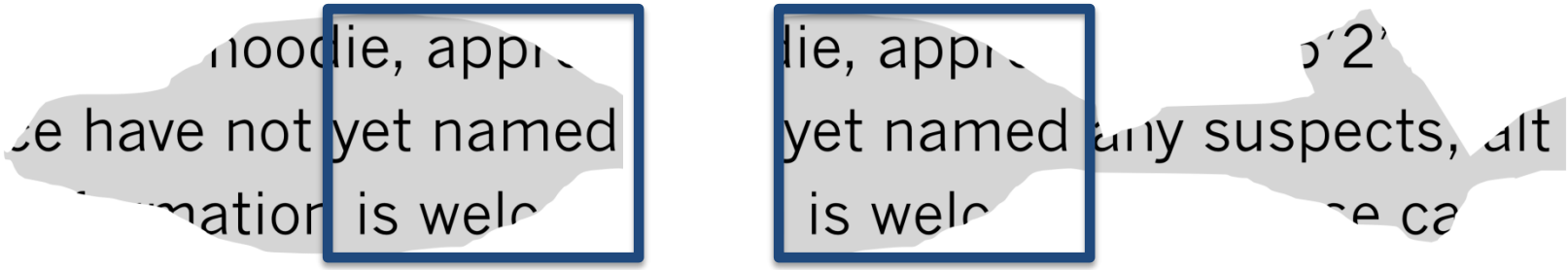




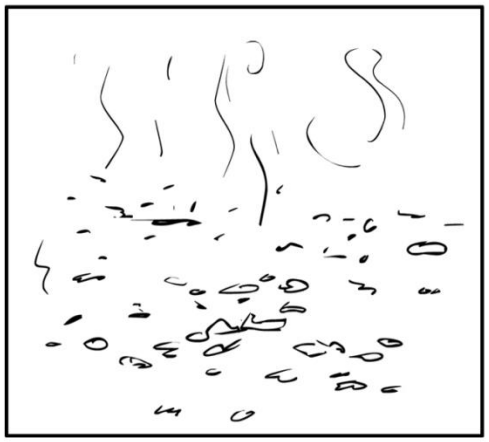
so, what did the June 27, 2000 NY
Times say?

The Newspaper Problem as an Overlapping Puzzle





The Newspaper Problem as an Overlapping Puzzle



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yet named any suspects, alt
is welc
e ca

Millions of Copies of a Genome

stack of NY Times, June 27, 2000

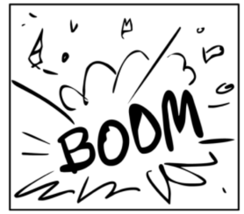
CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC

Breaking the Genomes at Random Positions



CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC
CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC
CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC
CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTACCACATCGTAGCTACGATGCATTAGCAAGCTATCGGATCAGCTACCACATCGTAGC

Generating Short Substring (Reads)

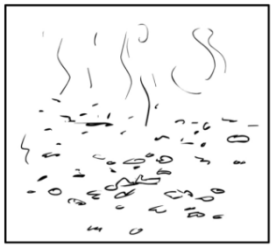
CTGATGA TGGACTACGCTAC TACTGCTAG CTGTATTACG ATCAGCTACCACA TCGTAGCTACG ATGCATTAGCAA GCTATCGGA TCAGCTACCA CATCGTAGC

CTGATGATG GACTACGCT ACTACTGCTA GCTGTATTACG ATCAGCTACC ACATCGTAGCT ACGATGCATTA GCAAGCTATC GGATCAGCTAC CACATCGTAGC

CTGATGATGG ACTACGCTAC TACTGCTAGCT GTATTACGATC AGCTACCAC ATCGTAGCTACG ATGCATTAGCA AGCTATCGG A TCAGCTACCA CATCGTAGC

CTGATGATGGACT ACGCTACTACT GCTAGCTGTAT TACGATCAGC TACCACATCGT AGCTACGATGCA TTAGCAAGCT ATCGGATCA GCTACCACATC GTAGC

Burning Some Reads



CTGATGA TGGACTACGCTAC TACTGCTAG CTGTATTACG ATCAGCTACCACA TCGTAGCTACG ATGCATTAGCAA GCTATCGGA TCAGCTACCA CATCGTAGC

CTGATGATG GACTACGCT ACTACTGCTA GCTGTATTACG ATCAGCTACC ACATCGTAGCT ACGATGCATTA GCAAGCTATC GGATCAGCTAC CACATCGTAGC

CTGATGATGG ACTACGCTAC TACTGCTAGCT GTATTACGATC AGCTACCAC ATCGTAGCTACG ATGCATTAGCA AGCTATCGG A TCAGCTACCA CATCGTAGC

CTGATGATGGACT ACGCTACTACT GCTAGCTGTAT TACGATCAGC TACCACATCGT AGCTACGATGCA TTAGCAAGCT ATCGGATCA GCTACCACATC GTAGC

Assembling Genome

CTGATGA TGGACTACGCTAC TACTGCTAG CTGTATTACG ATCAGCTACCACA TCGTAGCTACG ATGCATTAGCAA GCTATCGGA TCAGCTACCA CATCGTAGC

CTGATGATG GACTACGCT ACTACTGCTA GCTGTATTACG ATCAGCTACC ACATCGTAGCT ACGATGCATTA GCAAGCTATC GGATCAGCTAC CACATCGTAGC

CTGATGATGG ACTACGCTAC TACTGCTAGCT GTATTACGATC AGCTACCAC ATCGTAGCTACG ATGCATTAGCA AGCTATCGG A TCAGCTACCA CATCGTAGC

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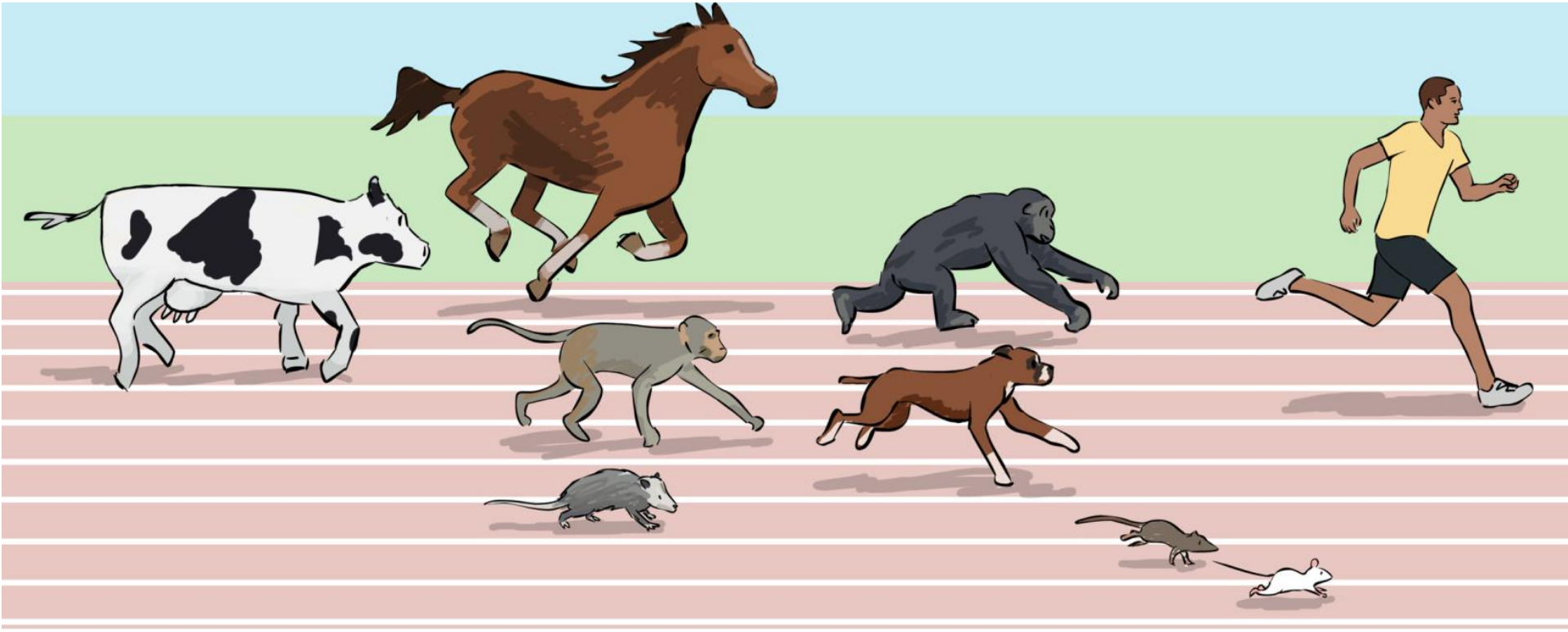
cow
2009
horse
2007
opossum
2007
macaque
2006
dog
2005
chimpanzee
2005
rat
2004
mouse
2002
human
2001

Why Do We Sequence 1000s of Species?

Applications in

- **medicine** (mouse genome)
- **agriculture** (rice genome)
- **biotechnology** (genomes of energy-producing bacteria),
- etc., etc., etc.

Few Mutations Can Make a Big Difference…

- Different people have slightly different genomes:
  on average, roughly 1 mutation in 1000 nucleotides.

- The 1 in 1000 nucleotides difference accounts for height, high cholesterol susceptibility, and 7000+ genetic diseases.

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGA
TCAGCTAC**C**ACATCGTAGCTACGATGCATTAGCAAGCTAT
CGATCGATCGATCGATTATCTACGATCGATCGATCGATCA
CTATACGAGCTACTACGTACGTACGATCGCG**G**GACTATTA
TCGACTACAGAT**A**AAACATGCTAGTACAACAGTATACATA
GCTGCGGGATACGATTAGCTAATAGCTGACGATATCCGAT

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGA
TCAGCTAC**A**ACATCGTAGCTACGATGCATTAGCAAGCTAT
CGATCGATCGATCGATTATCTACGATCGATCGATCGATCA
CTATACGAGCTACTACGTACGTACGATCGCG**T**GACTATTA
TCGACTACAGAT**G**AAACATGCTAGTACAACAGTATACATA
GCTGCGGGATACGATTAGCTAATAGCTGACGATATCCGAT

Emergence of Personalized Medicine

- **2010:** Nicholas Volker became the first child to be saved by genome sequencing.
  - Doctors could not diagnose his condition; he went through dozens of surgeries.
  - Sequencing revealed a mutation in a gene linked to a defect in his immune system.
  - This led doctors to use immunotherapy, which saved the child.

From Reference Genome to Personal Genomes

- **Reference human genome** assembled in 2000.

CTGAGGATGGACTACGCTACTACTGATAGCTGTTT

reference genome

GAGGA CCACG TGA-AG

CTGA GGACC ACTAC A-AGCT

GATGG ACGCT TGTTT

reads

CTGAGGATGGACCACGCTACTACTGA-AGCTGTTT

personal genome

Exact Pattern Matching

- Where does a read match the reference genome *exactly*?

- **Pattern Matching Problem:**
  - **Input:** A string *Pattern* (read) and a string *Text* (genome).
  - **Output:** All positions in *Text* where *Pattern* appears as a substring.

Approximate Pattern Matching

- Where does a read match the reference genome *approximately*?

- **Approximate Pattern Matching Problem:**
  - **Input:** A string *Pattern*, a string *Text,* and an integer *d*
  - **Output:** All positions in *Text* where *Pattern* appears as a substring with at most *d* mismatches.

Multiple Pattern Matching

- Where do billions of reads match the reference genome?

- **Multiple Pattern Matching Problem:**
  - **Input:** A set of strings *Patterns* and a string *Text.*
  - **Output:** All positions in *Text* where a string from *Patterns* appears as a substring.

Outline

- From Genome Sequencing to Pattern Matching
- **Brute Force Approach to Pattern Matching**
- Herding Patterns into Trie
- Herding Text into Suffix Trie
- From Suffix Tries to Suffix Trees

A Brute Force Approach to Exact Pattern Matching

Genome

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTAC**C**ACATCGTAGCTAC

Pattern drives along *Text*

p a n a m a b a n a n a s *Text*

n a n a *Pattern*

p a n a m a b a n a n a s

n a n a

Text

Pattern

p a n a m a b a n a n a s *Text*

n a n a *Pattern*

p a **n** a m a b a n a n a s *Text*

n a n a *Pattern*

p a **n a** m a b a n a n a s

n a n a

Text

Pattern

p a **n a m** a b a n a n a s *Text*

n a n a *Pattern*

p a n **a** m a b a n a n a s

n a n a

Text

Pattern

p a n a **m** a b a n a n a s

n a n a

Text

Pattern

p a n a m **a** b a n a n a s

Text

n a n a

Pattern

p a n a m a **b** a n a n a s

n a n a

Text

Pattern

p a n a m a b **a** n a n a s *Text*

n a n a *Pattern*

p a n a m a b a **n** a n a s *Text*

n a n a *Pattern*

p a n a m a b a **n a** n a s *Text*

n a n a *Pattern*

p a n a m a b a **n a n** a s *Text*

n a n a *Pattern*

Pattern Found!

p a n a m a b a **n a n a** s *Text*

n a n a *Pattern*

p a n a m a b a n **a** n a s *Text*

n a n a *Pattern*

Brute Force Approach Is Fast!

- **single** *Pattern*: $O(|Text| \cdot |Pattern|)$

The runtime of the **Knuth-Morris-Pratt** algorithm: $O(|Text|)$

(wait for the lecture on algorithmic challenges in pattern matching)

Brute Force Approach is Slow for **Billions** of Patterns

- **single** *Pattern*: $O(|Text| \bullet |Pattern|)$
- **multiple** *Patterns*:

$$O\left(\sum_{\substack{\text{all strings } Pattern \\ \text{In } Patterns}} |Text| \bullet |Pattern|\right)$$

Brute Force Approach is Slow for Billions of Patterns

- **single** *Pattern*: $O(|Text| \bullet |Pattern|)$
- **multiple** *Patterns*:

$$O\left(\sum_{\substack{\text{all strings } Pattern \\ \text{In } Patterns}} |Text| \bullet |Pattern|\right) =$$

$$O(|Text| \bullet |Patterns|)$$

For human genome:

- $|Text| \approx 3*10^9$
- $|Patterns| \approx 10^{12}$

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- Herding Text into Suffix Trie
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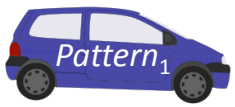
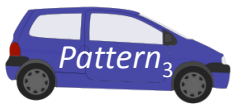
Patterns Travel One at a Time

Genome

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTAC**C**ACATCGTAGCTAC

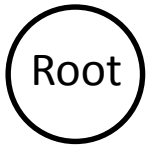




Herding Patterns onto a Bus

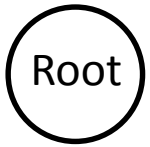
Genome

CTGATGATGGACTACGCTACTACTGCTAGCTGTATTACGATCAGCTAC**C**ACATCGTAGCTAC



Patterns

banana
pan
nab
antenna
bandana
ananas
nana



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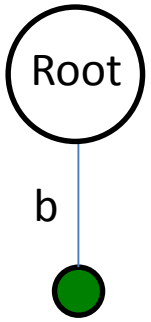

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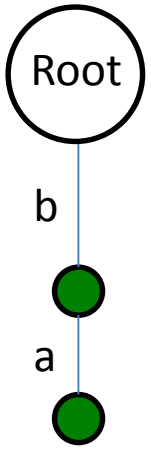

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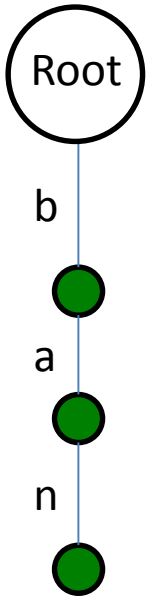

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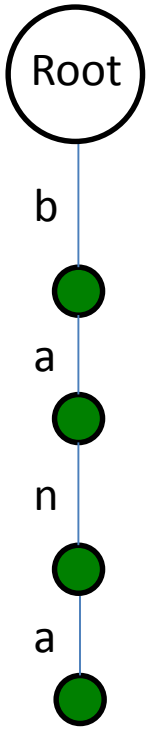

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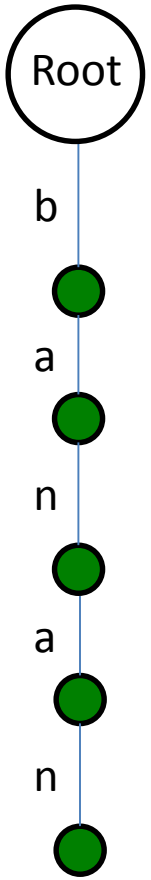

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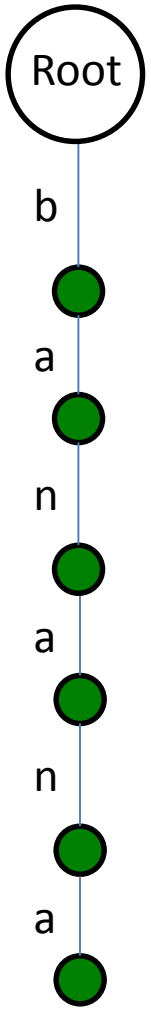

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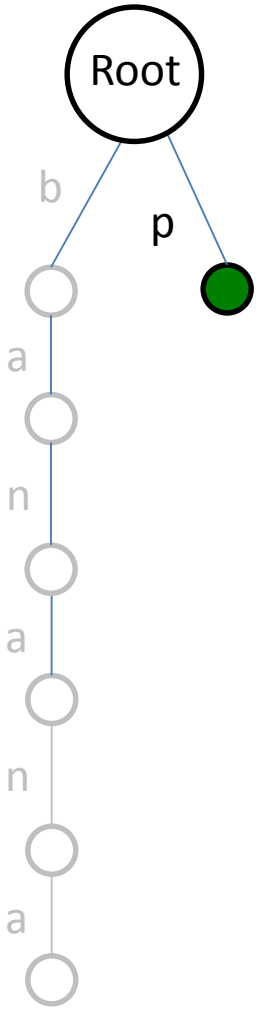

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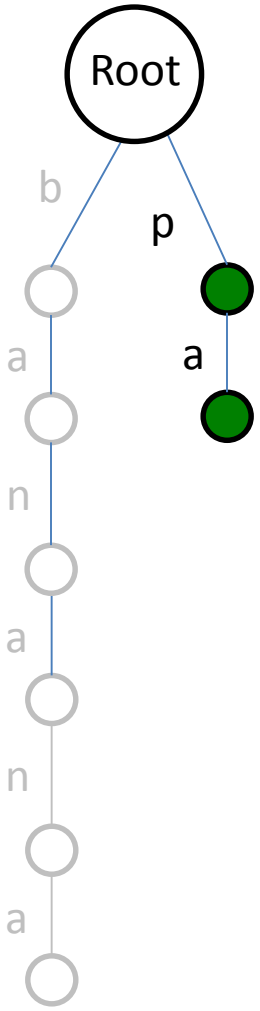

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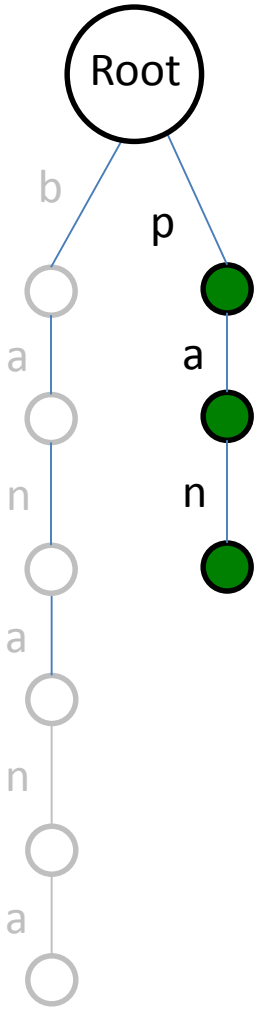

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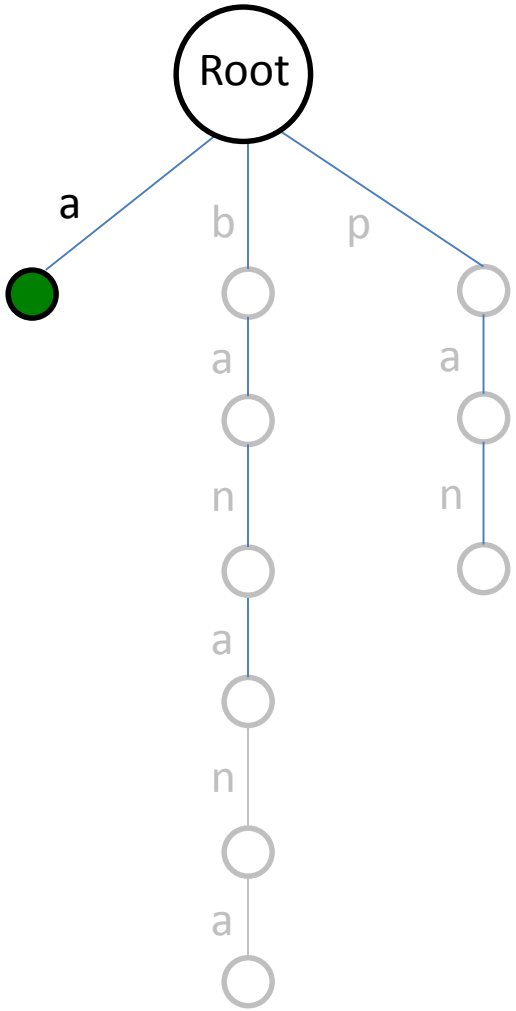

Patterns

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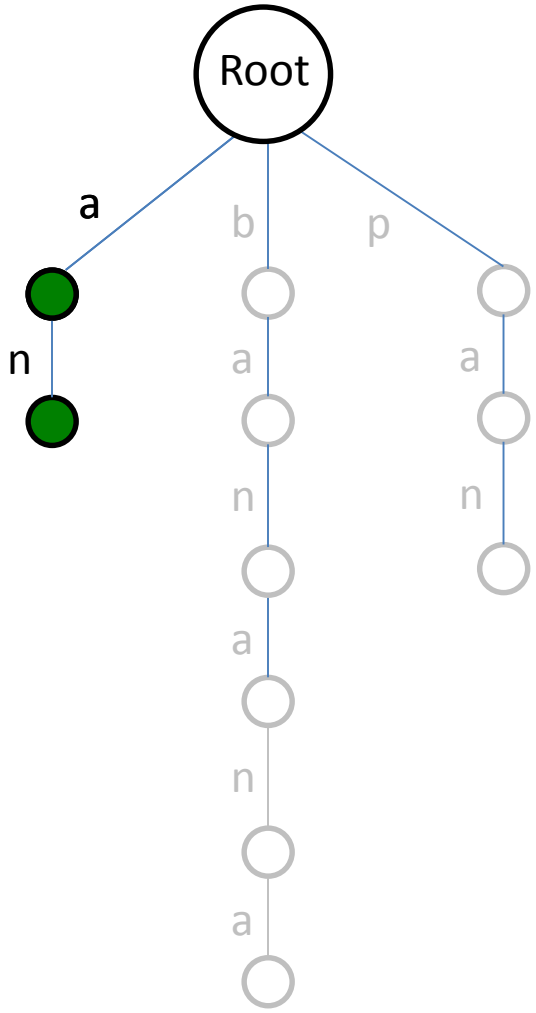

Patterns

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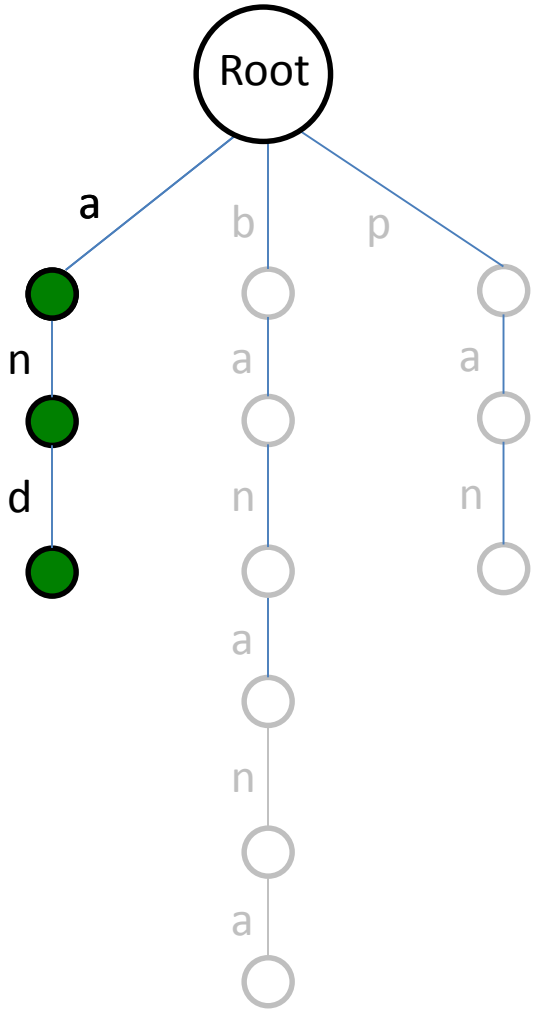

Patterns

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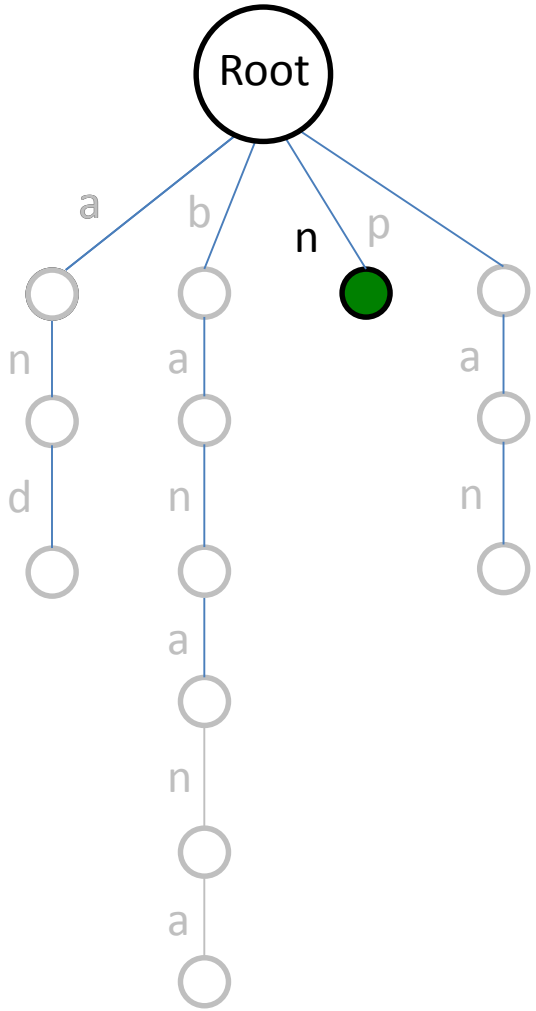

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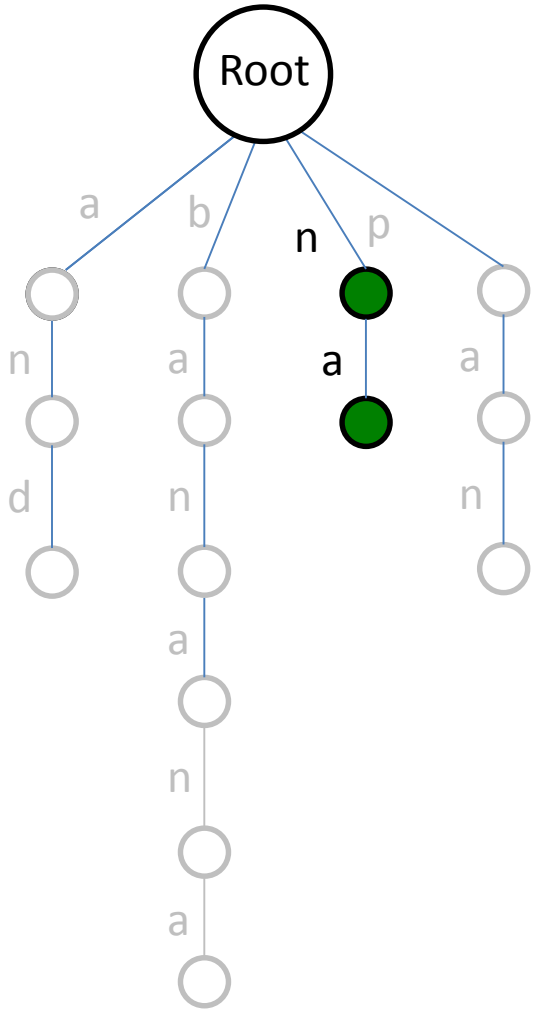

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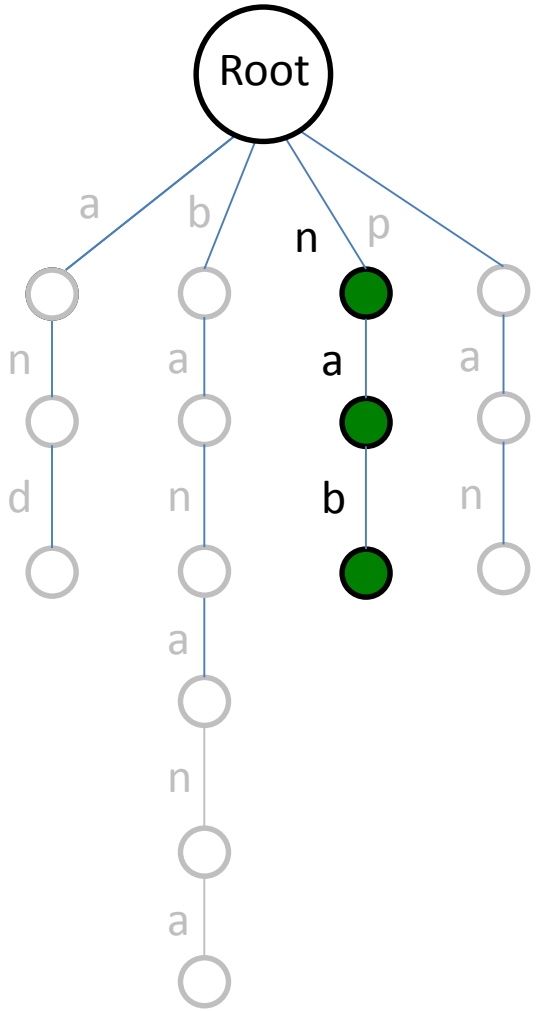

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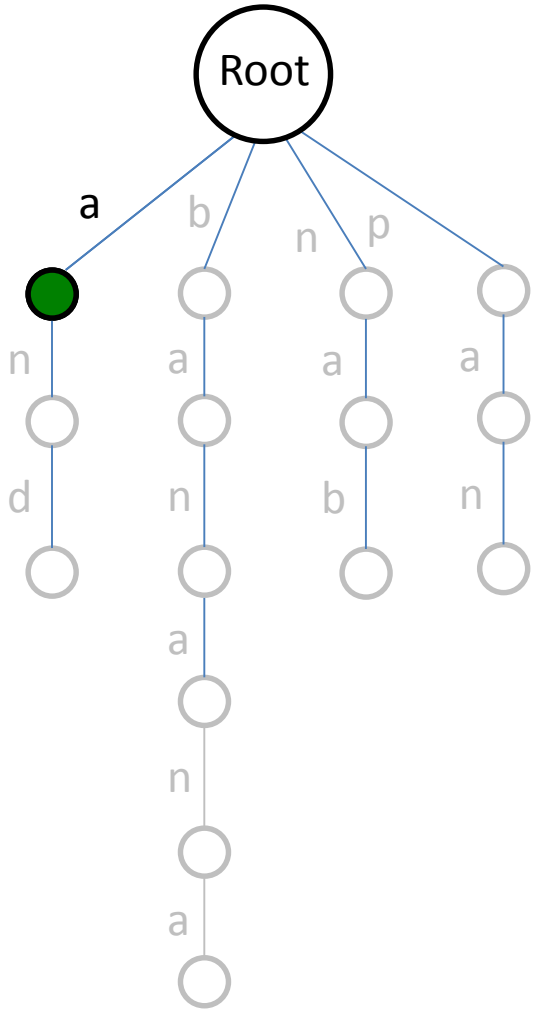

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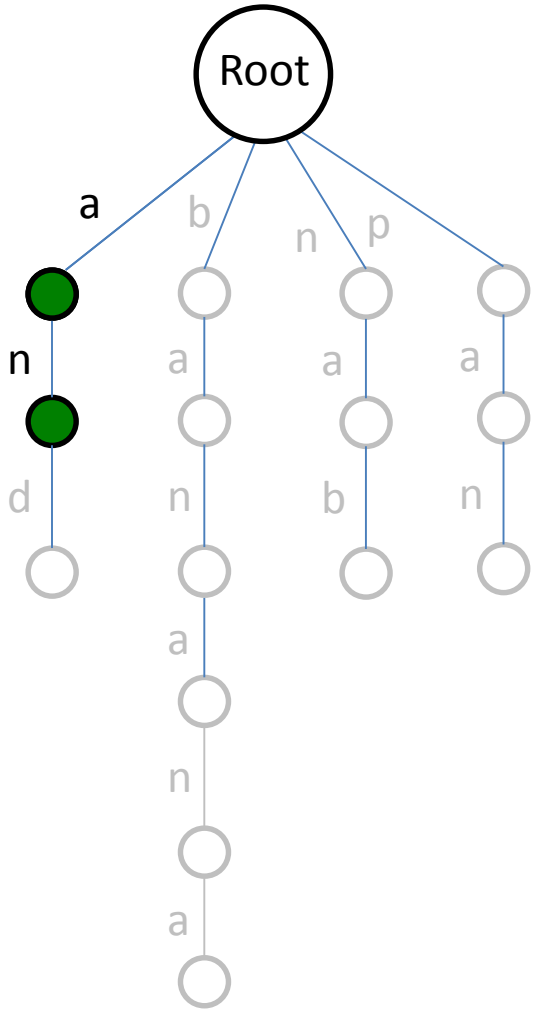

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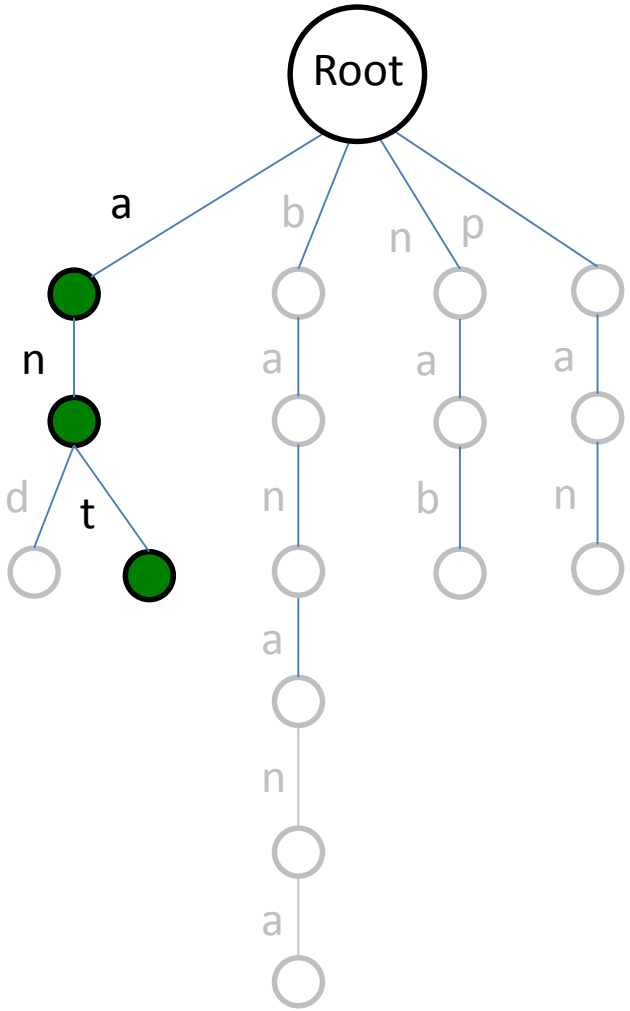

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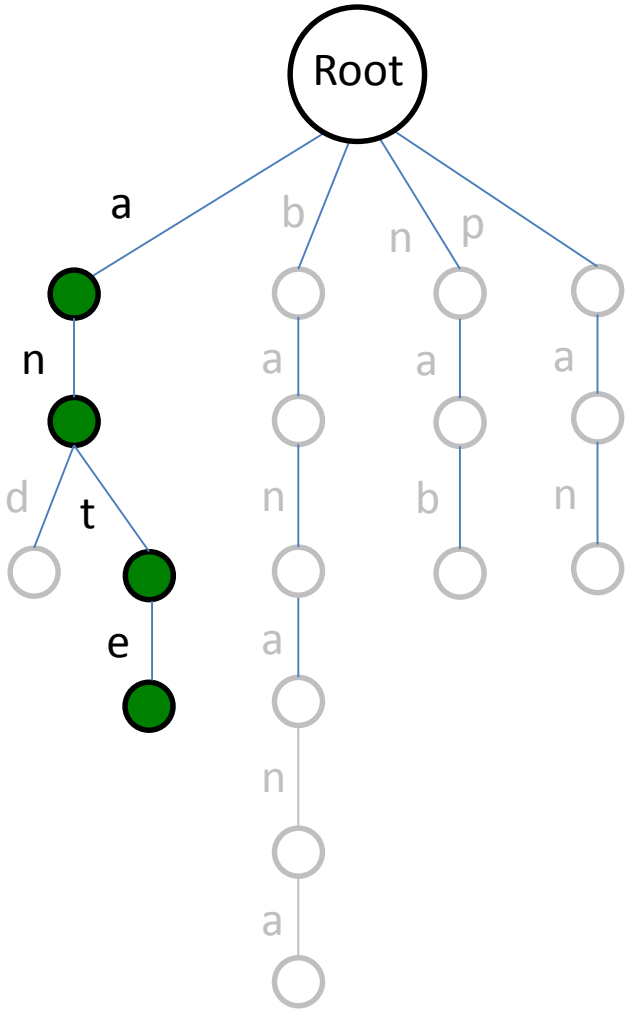

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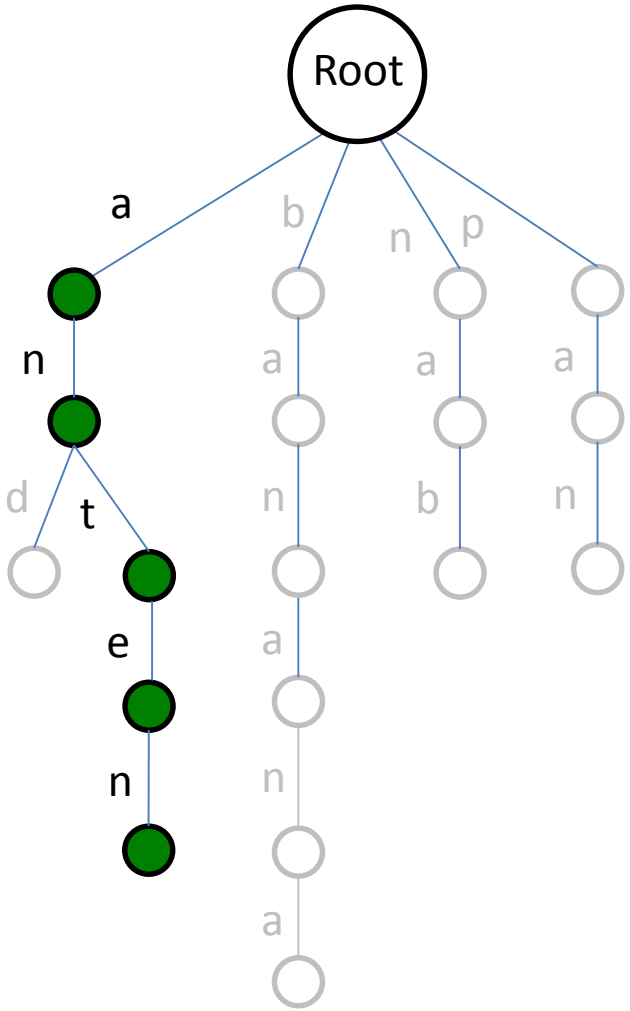

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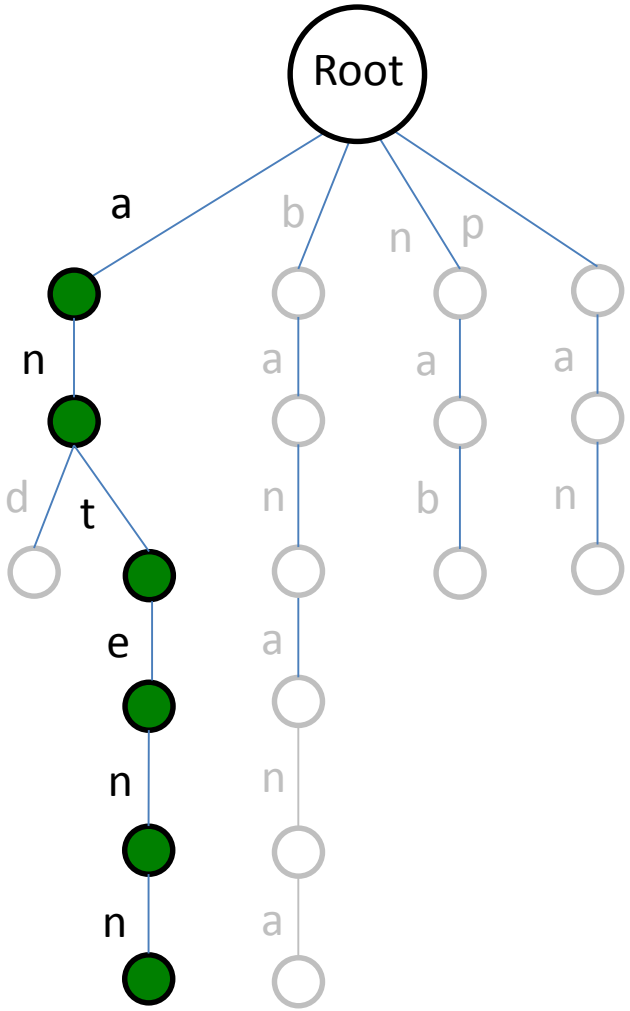

Patterns

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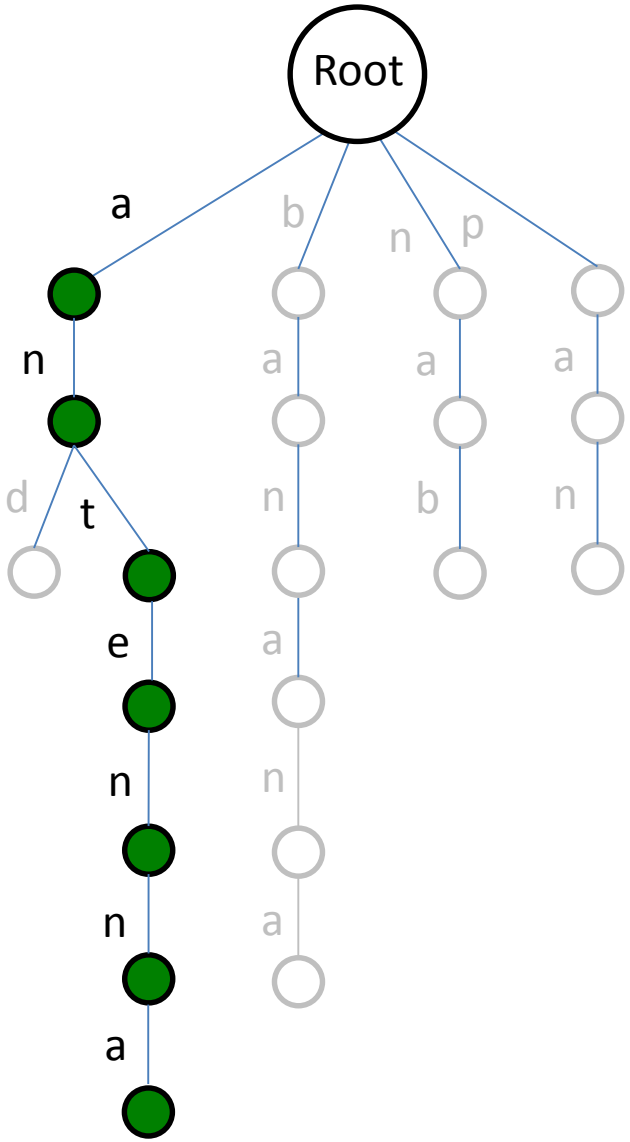

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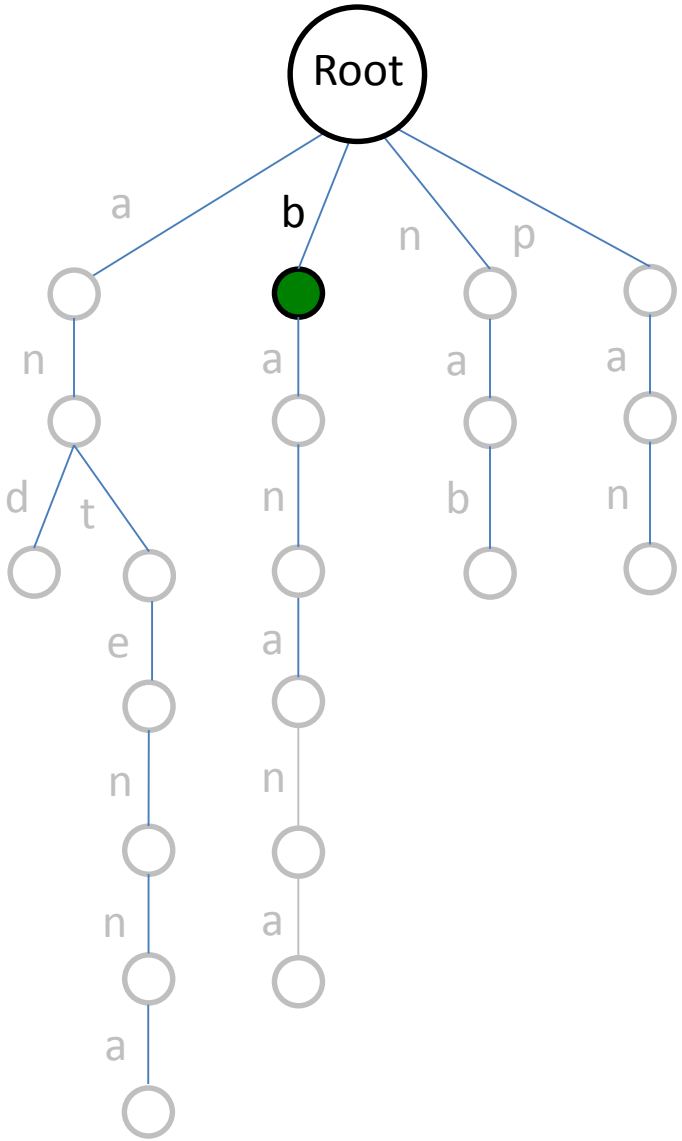

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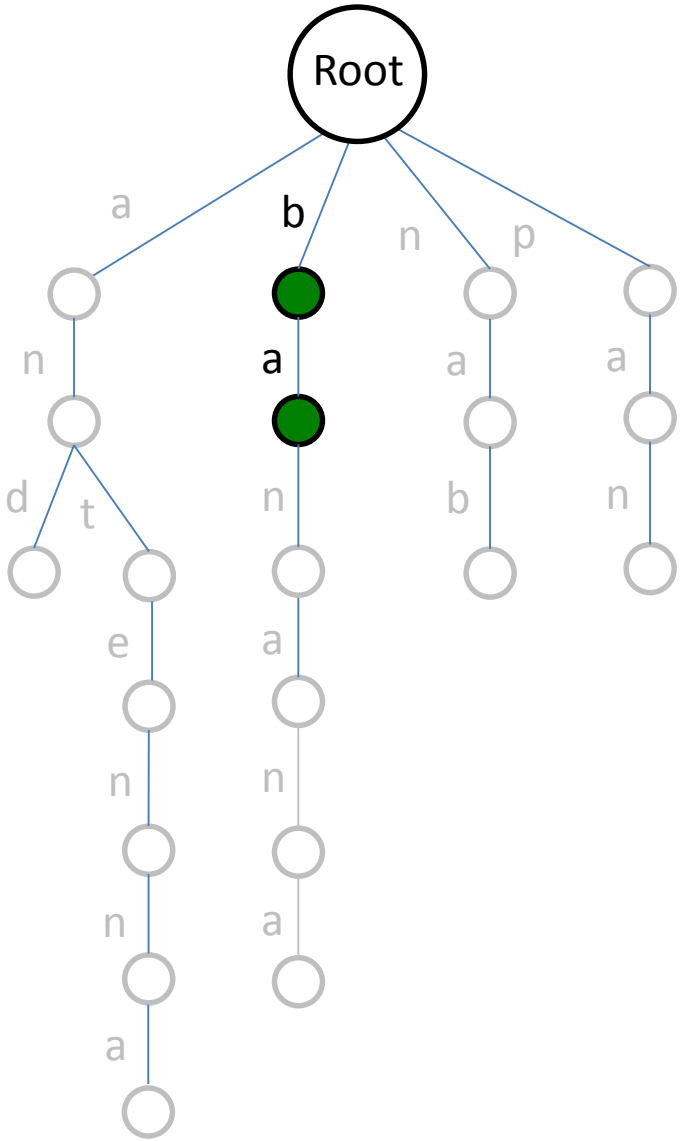

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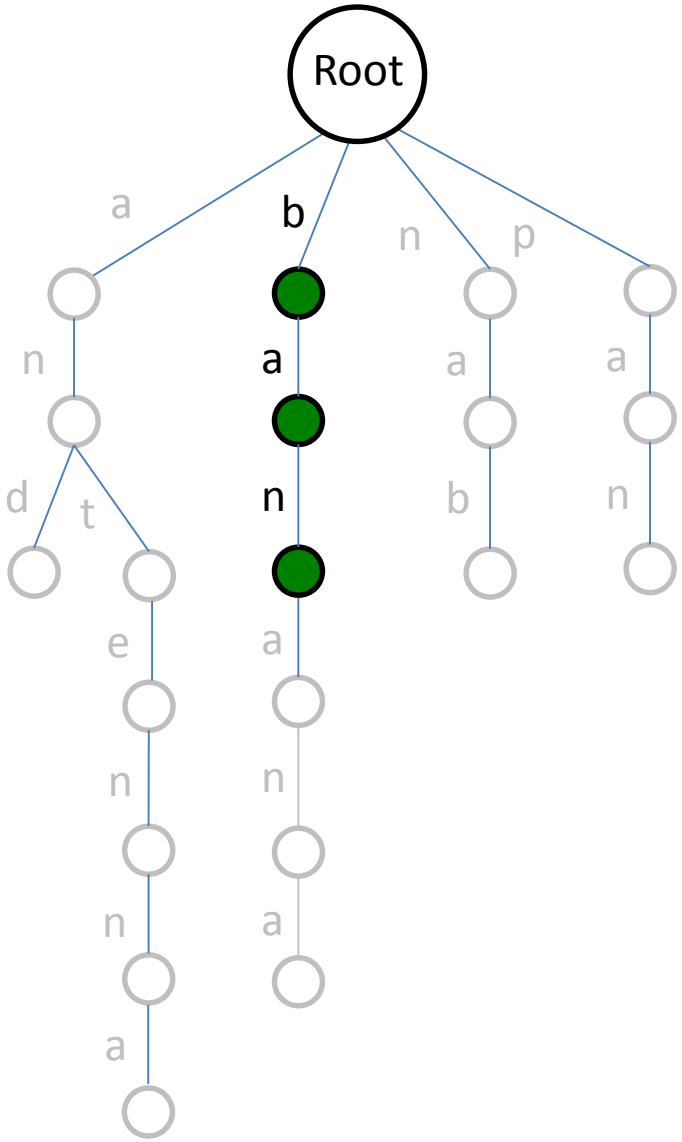

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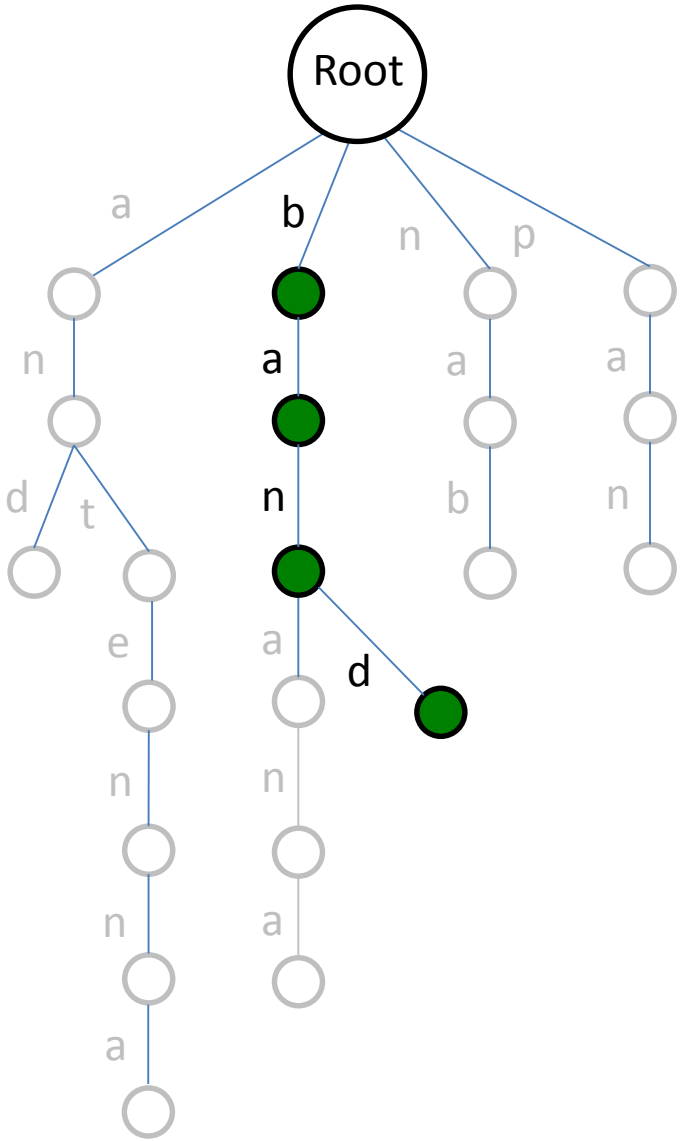

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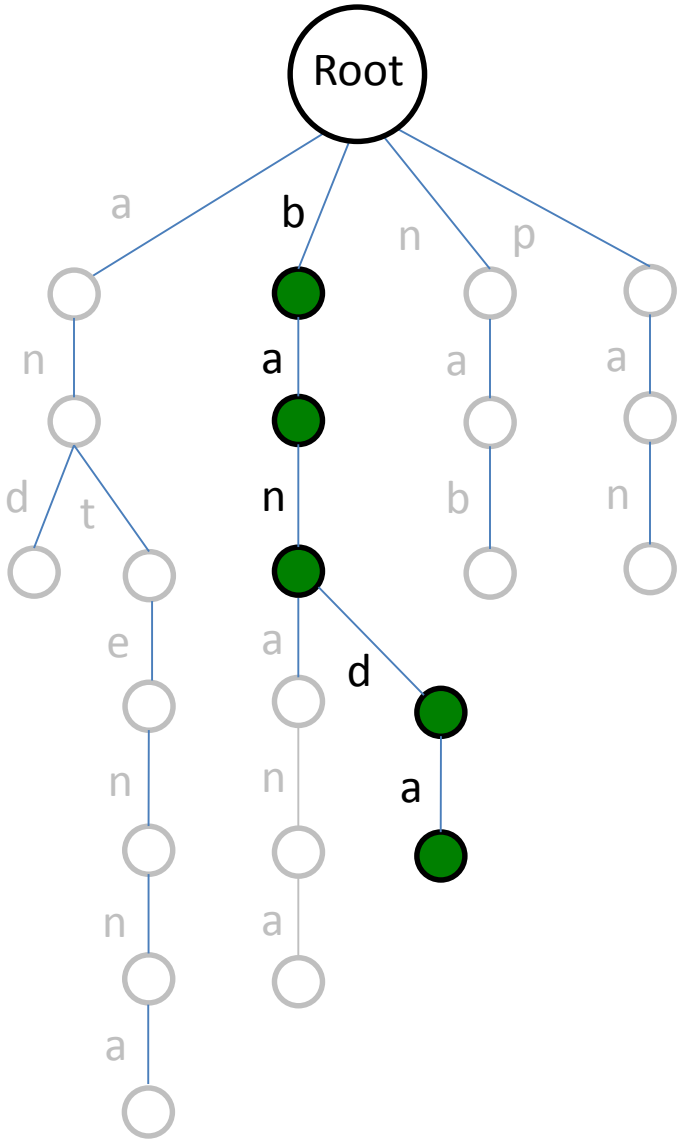

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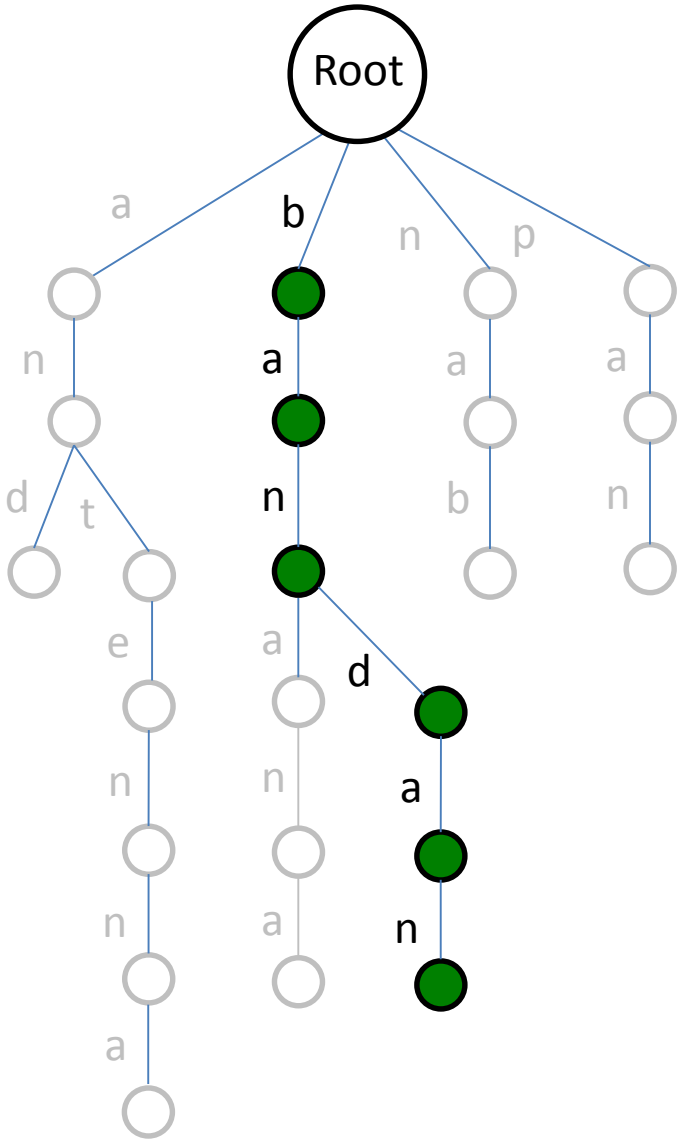

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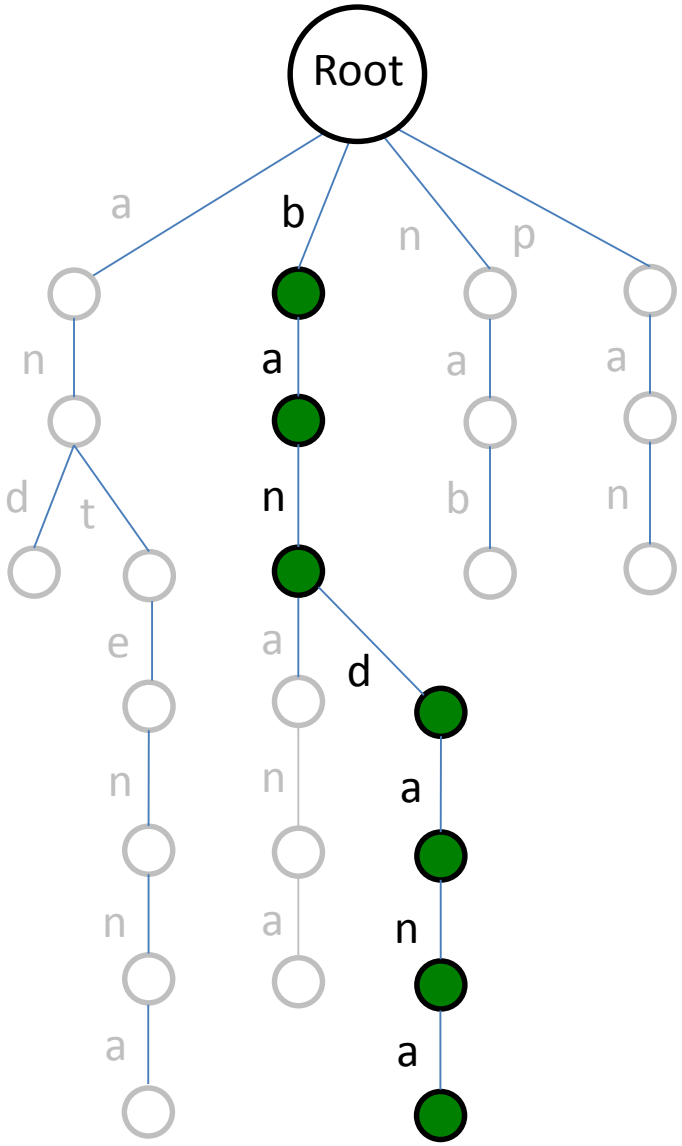

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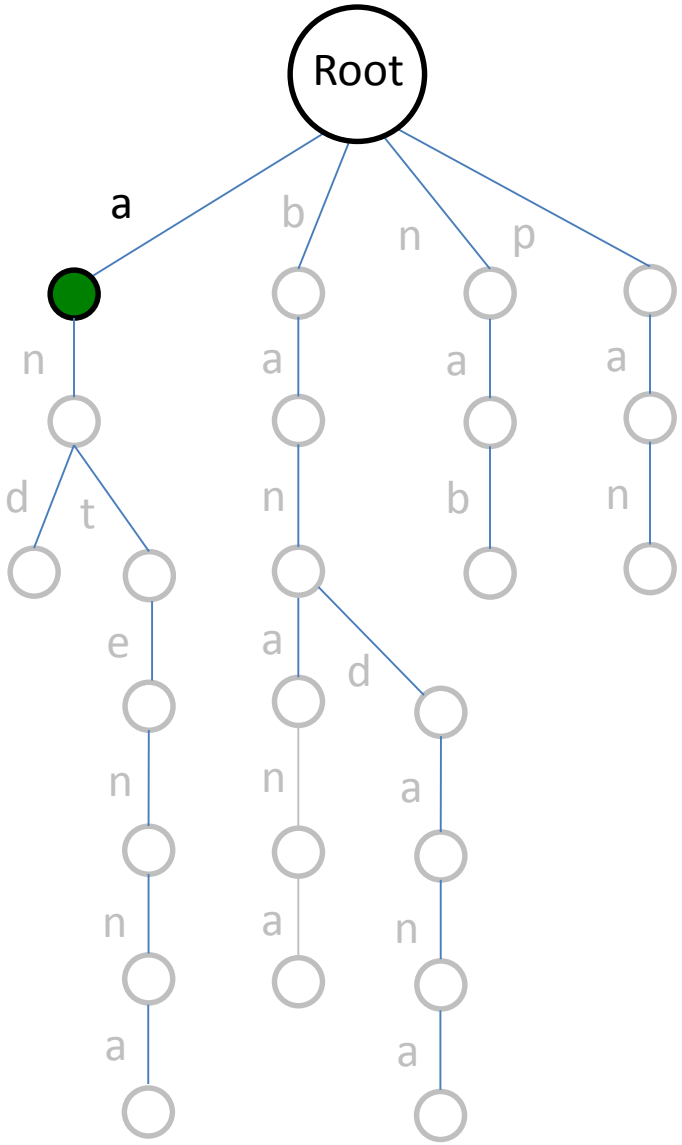

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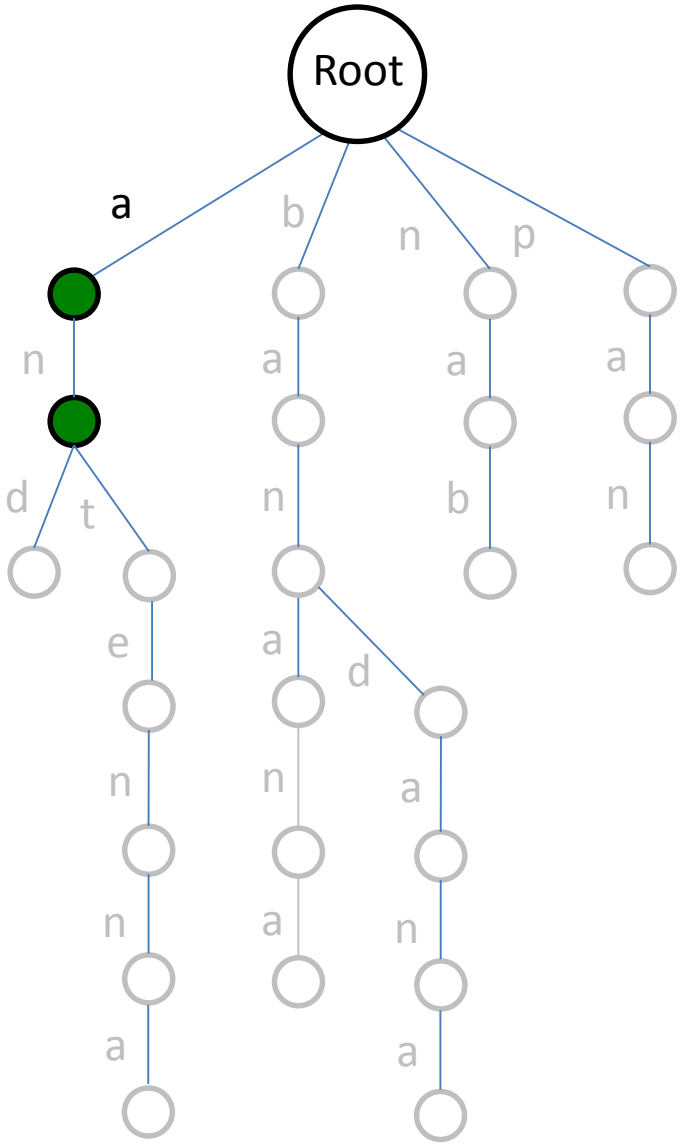

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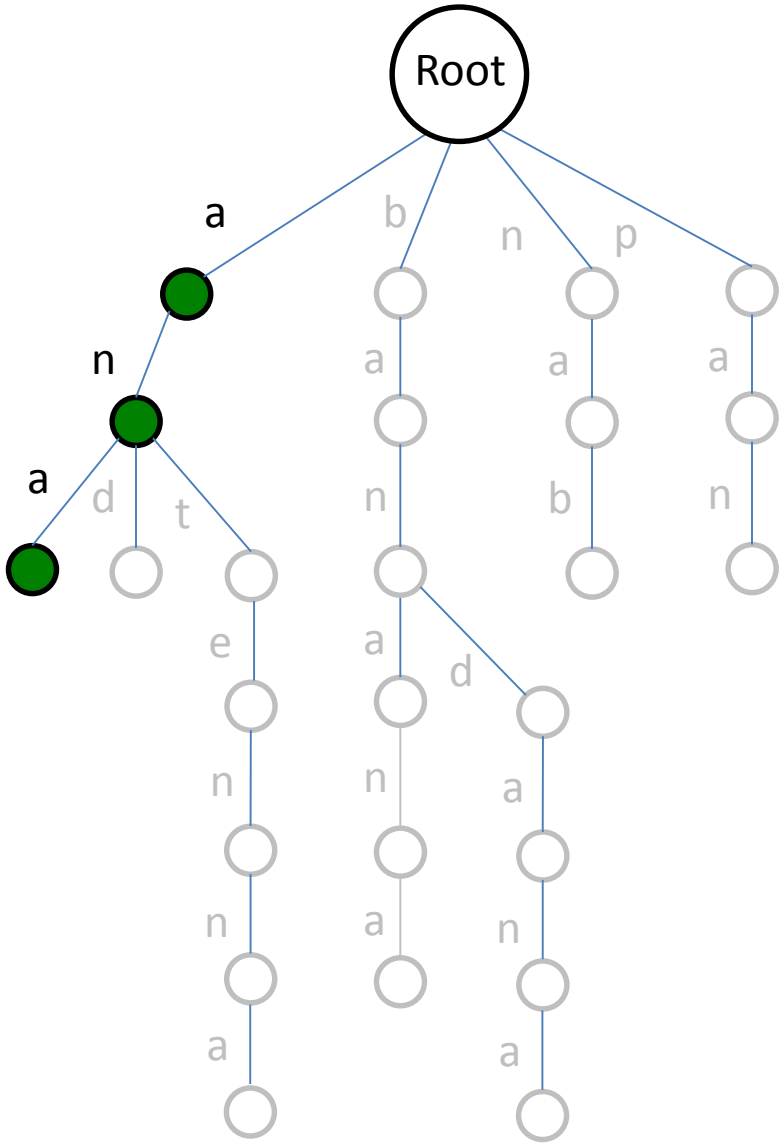

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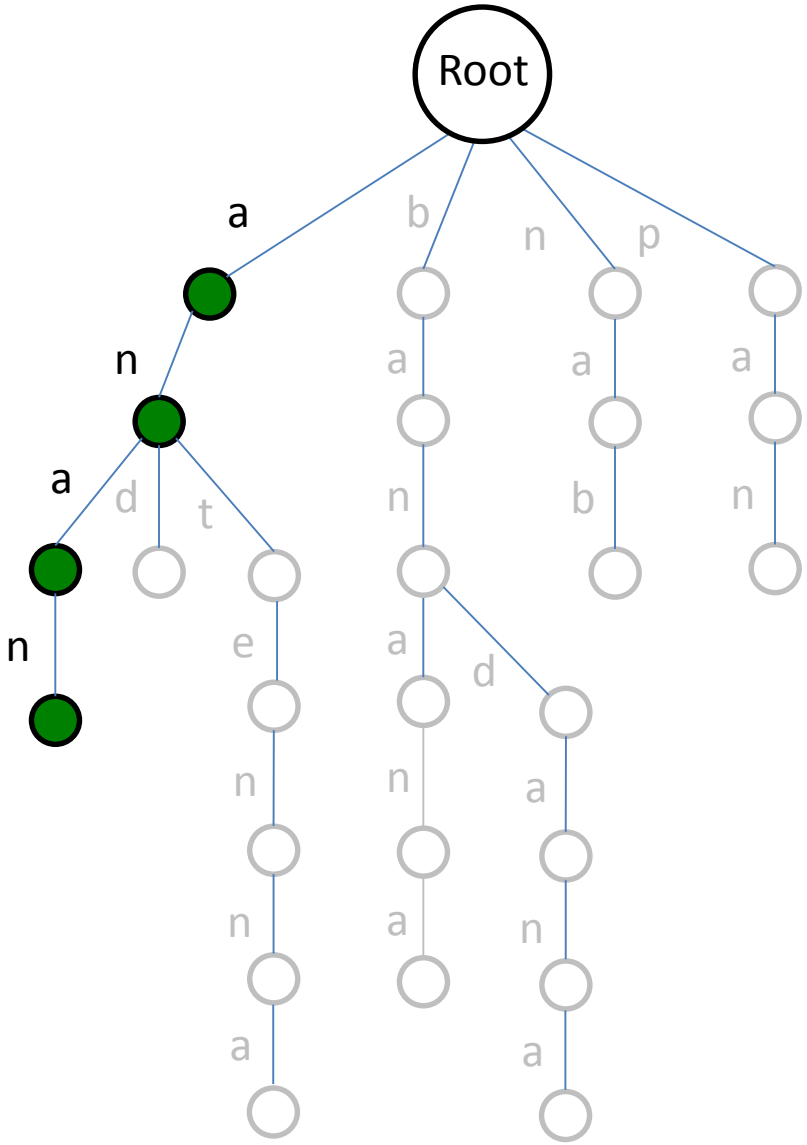

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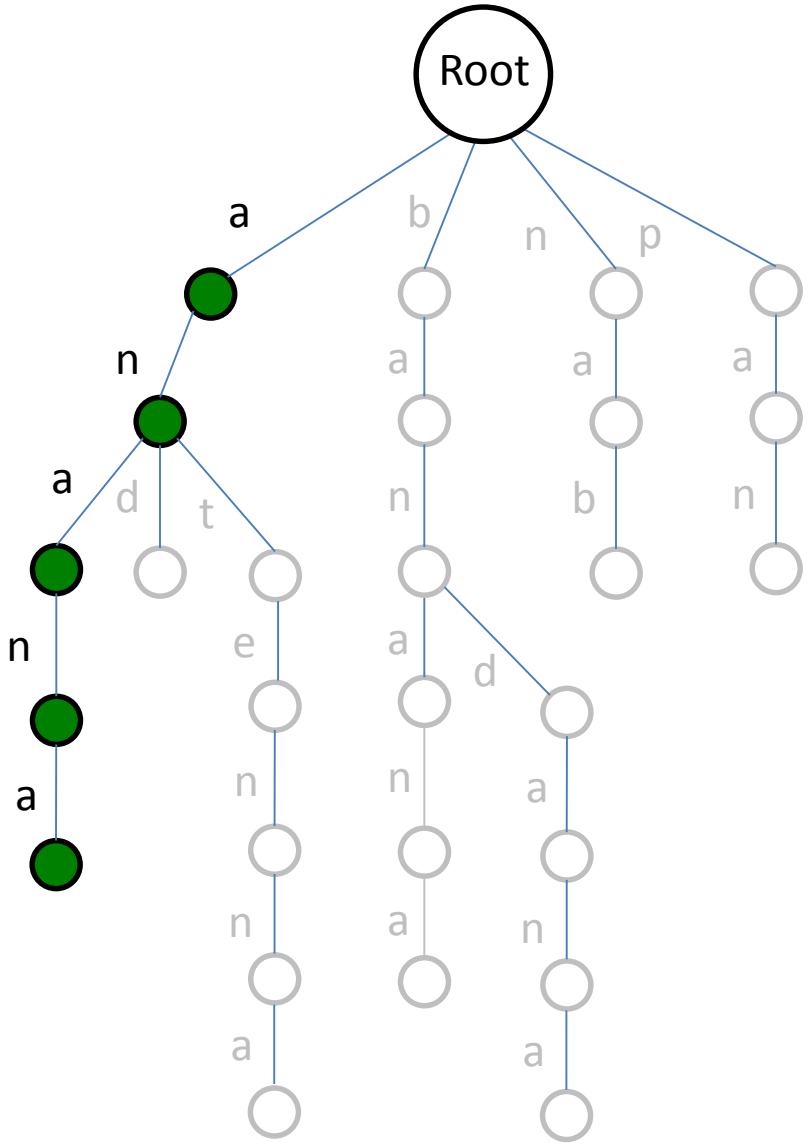

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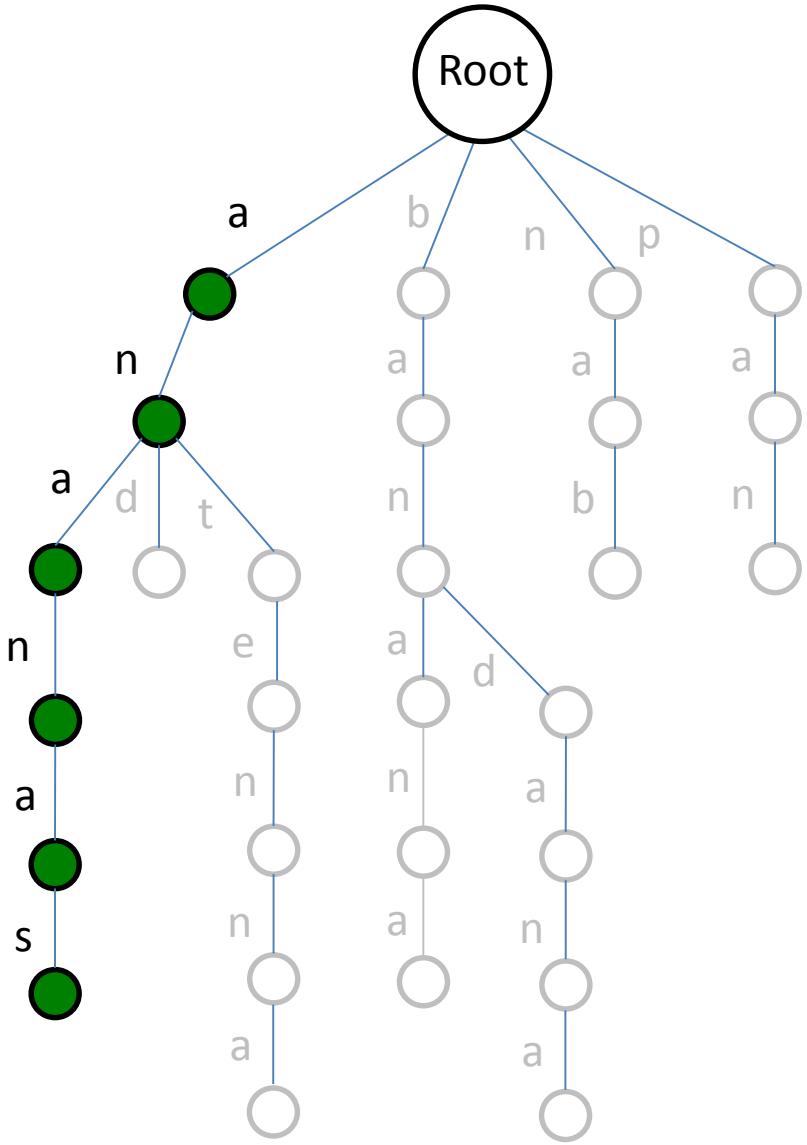

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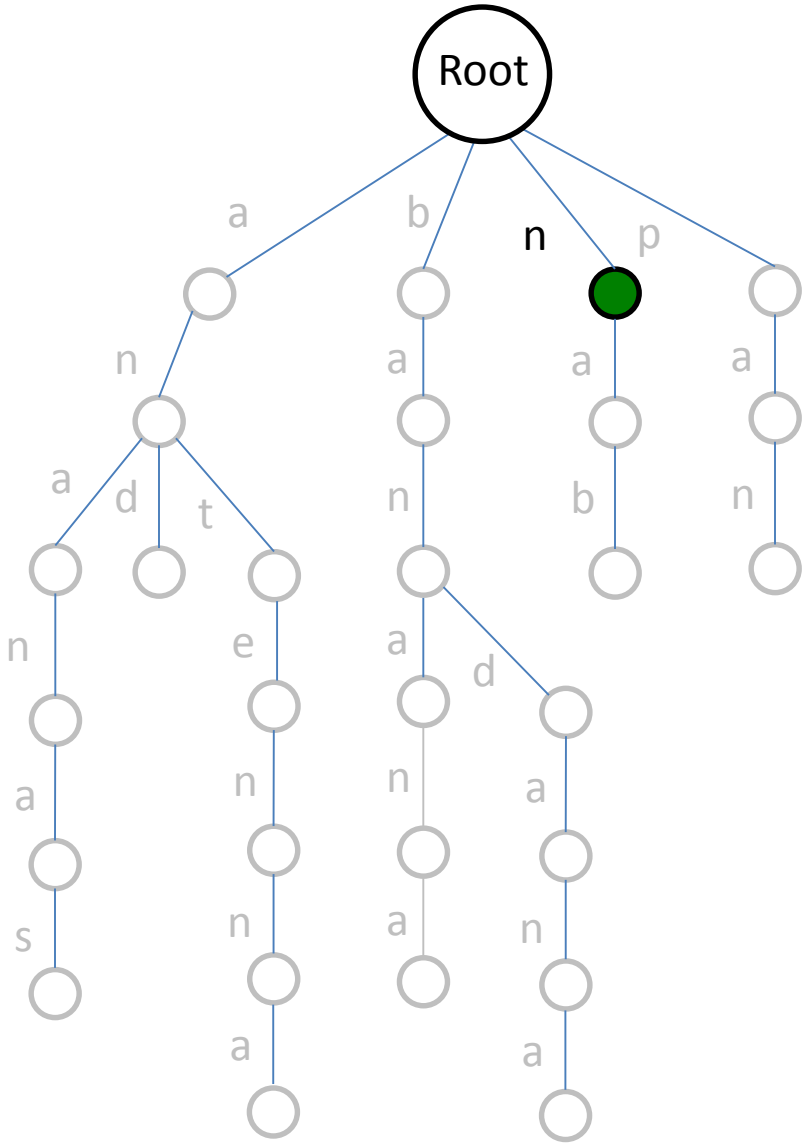

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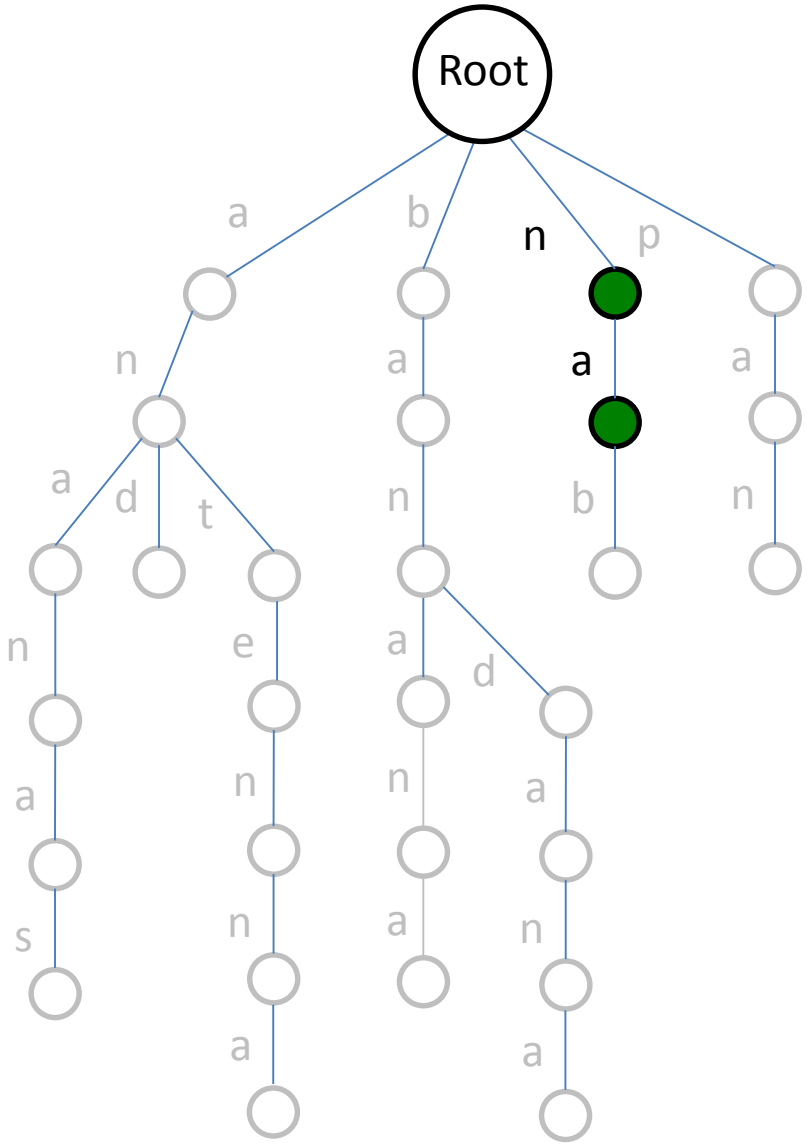

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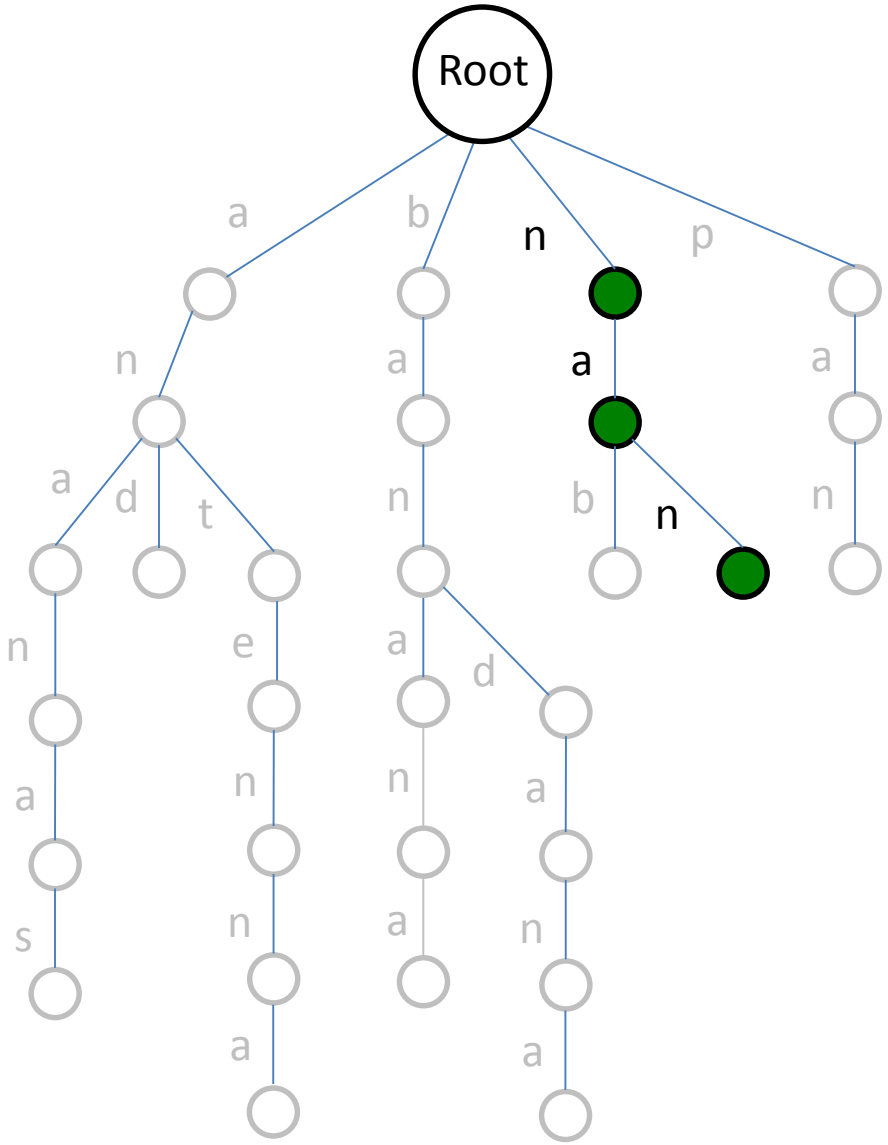

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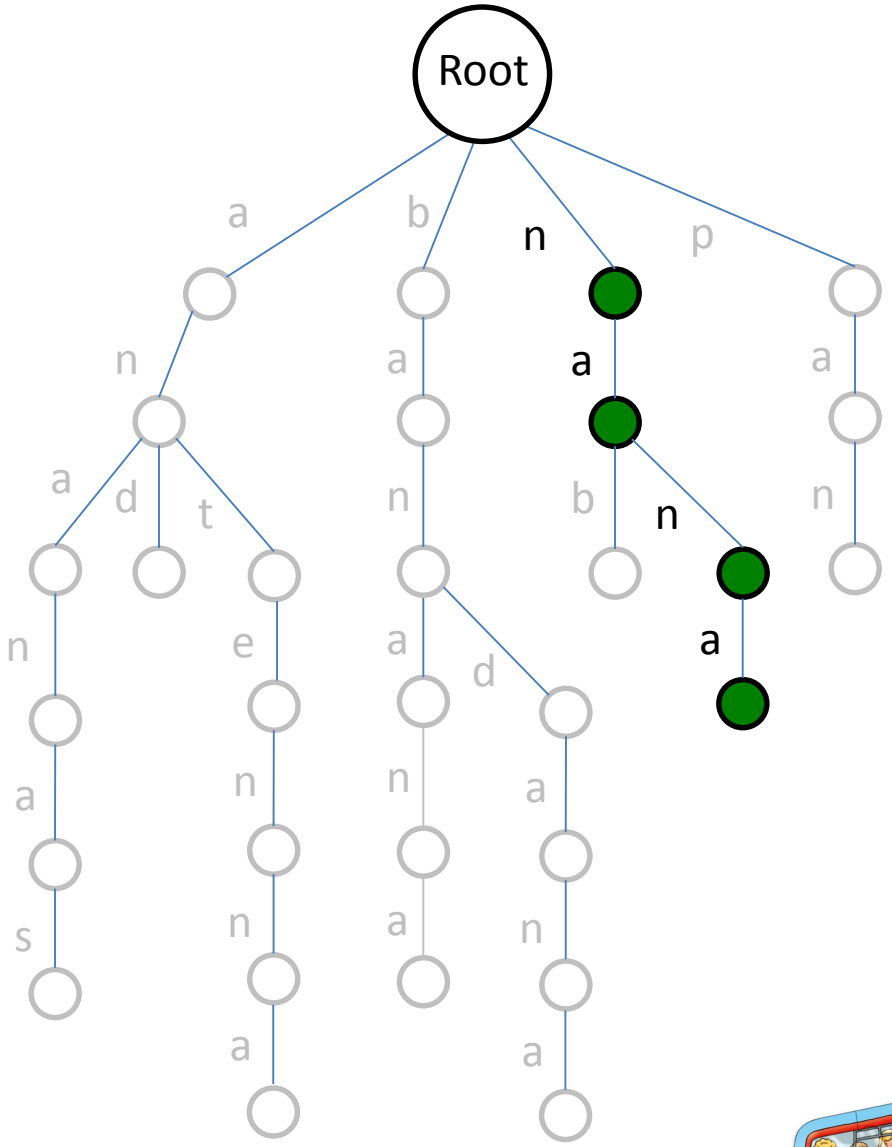

Trie(*Patterns*)

Patterns

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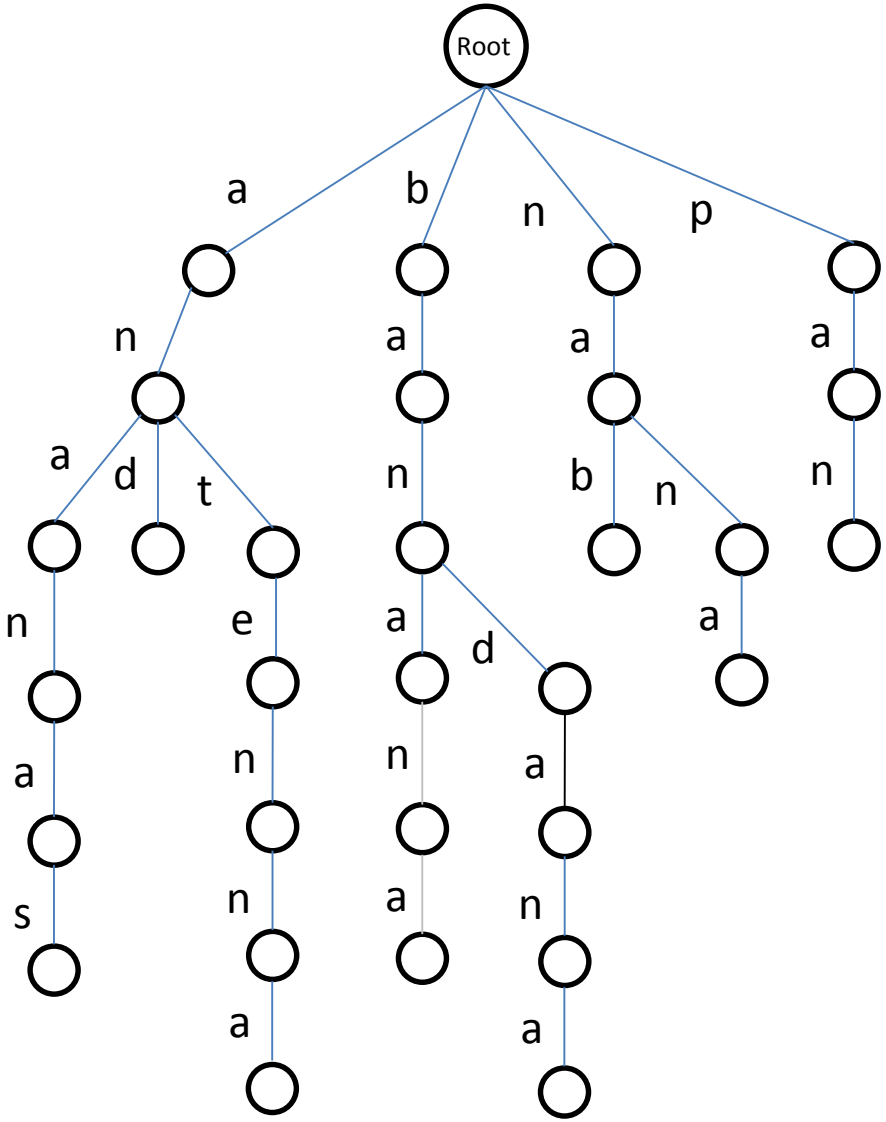
p a n a m a b a n a n a s



TrieMatching(*Text, Patterns*):

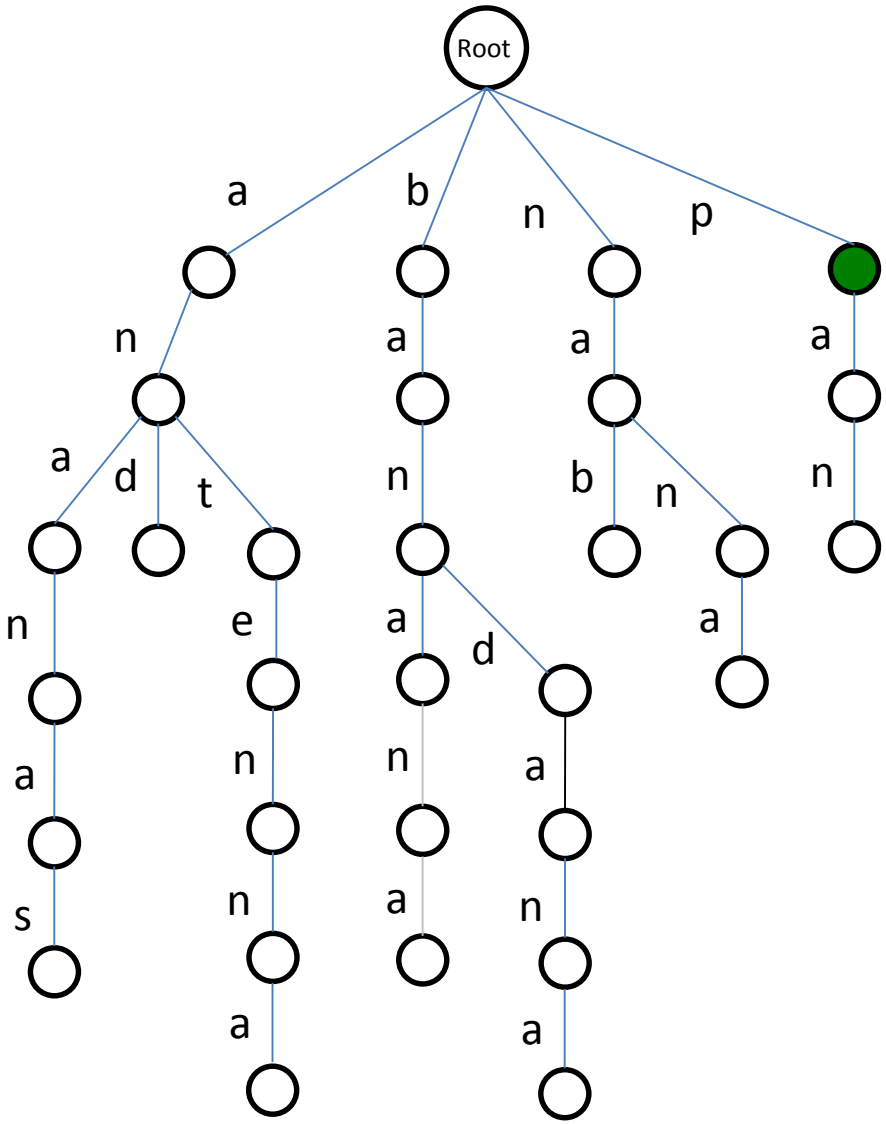
drive Trie(*Patterns*) along *Text*

at each position of *Text*

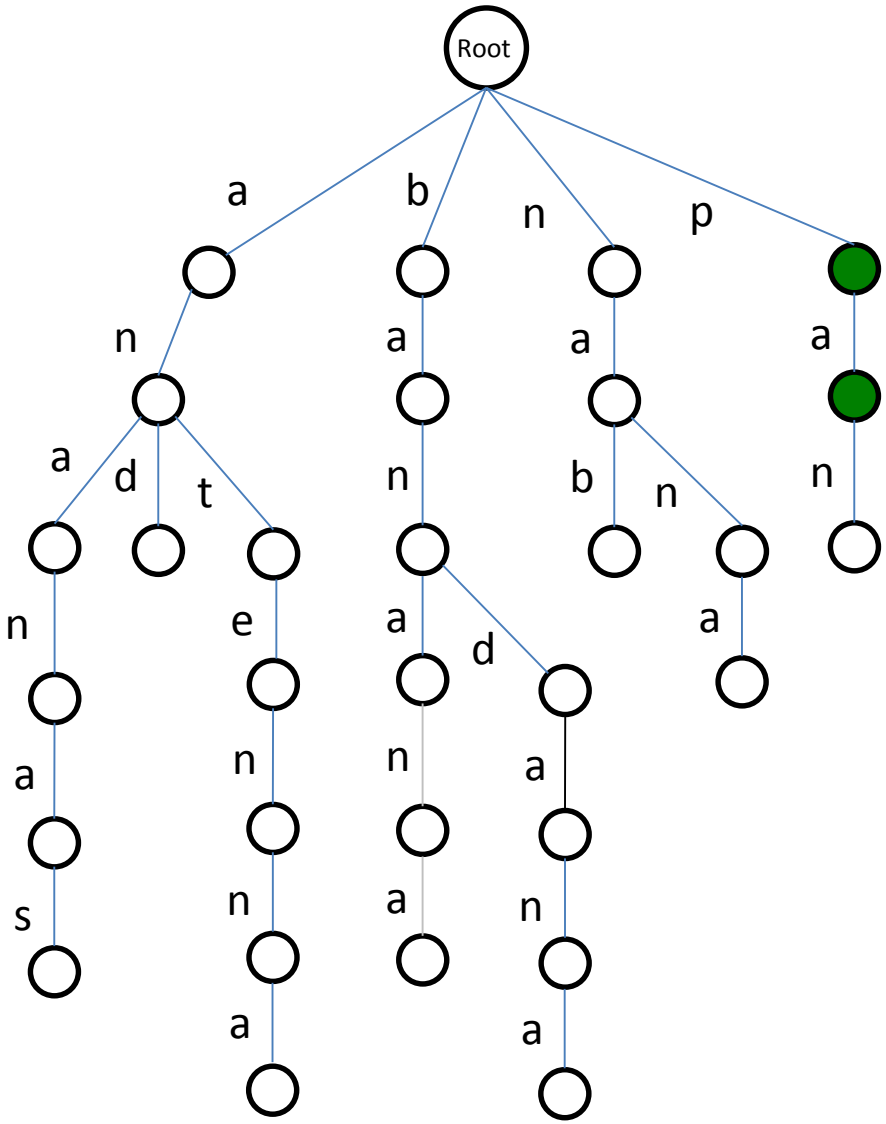
- walk down Trie(*Patterns*) by spelling symbols of *Text*
- a pattern from *Patterns* matches *Text* each time you reach a leaf!

For simplicity, we assume that no pattern is a substring of another pattern

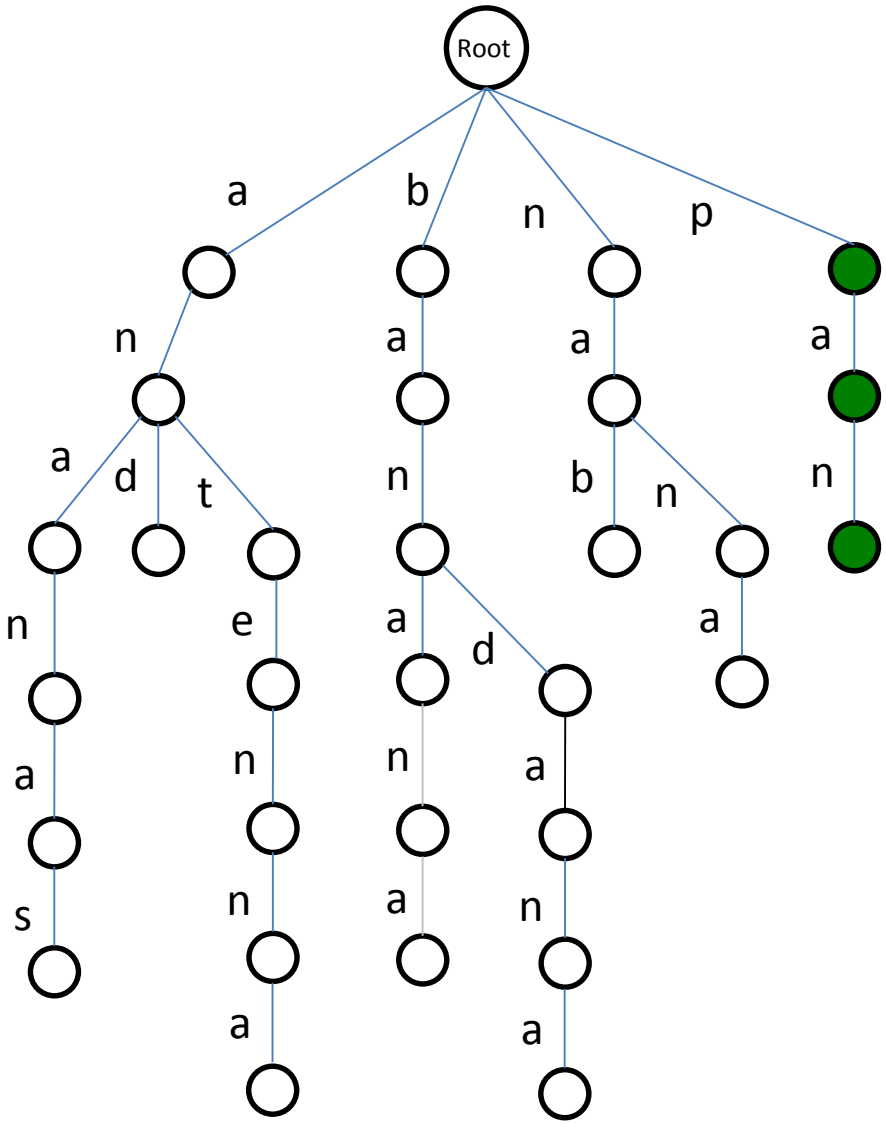
p a n a m a b a n a n a s



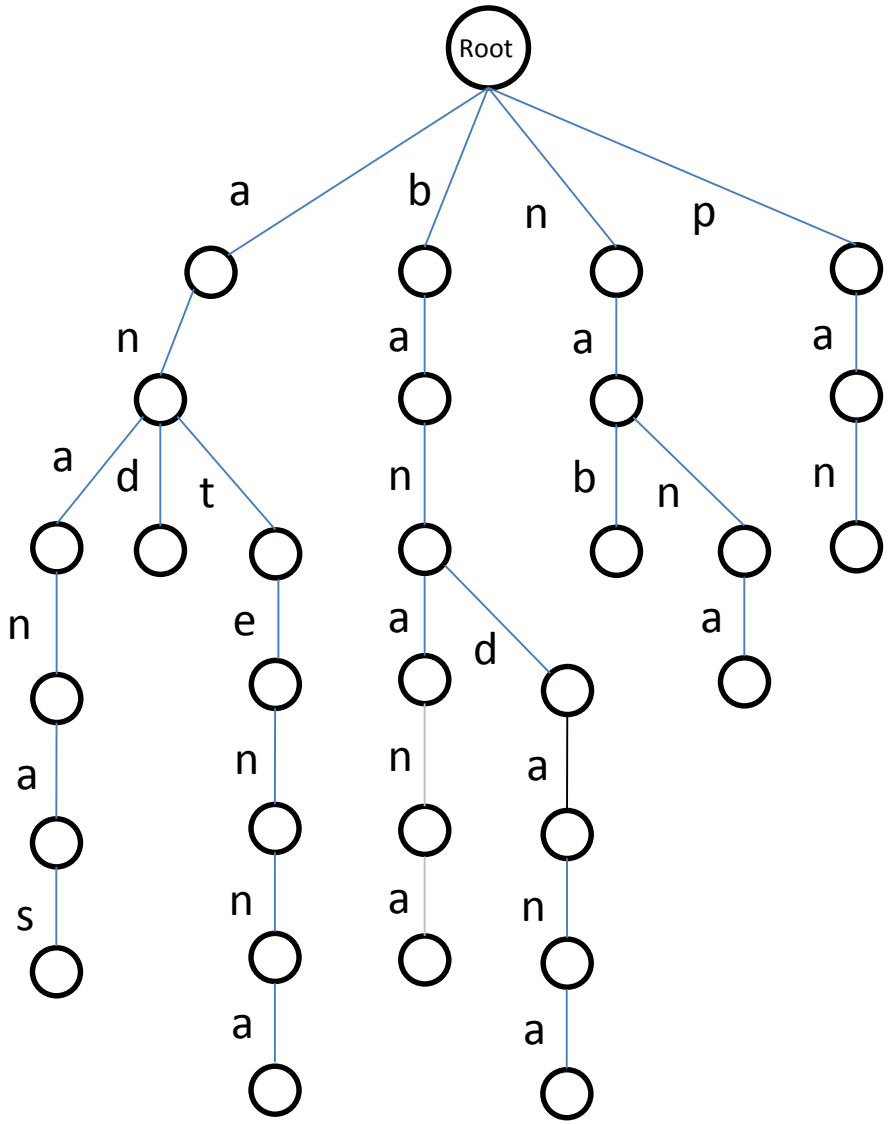
p a n a m a b a n a n a s



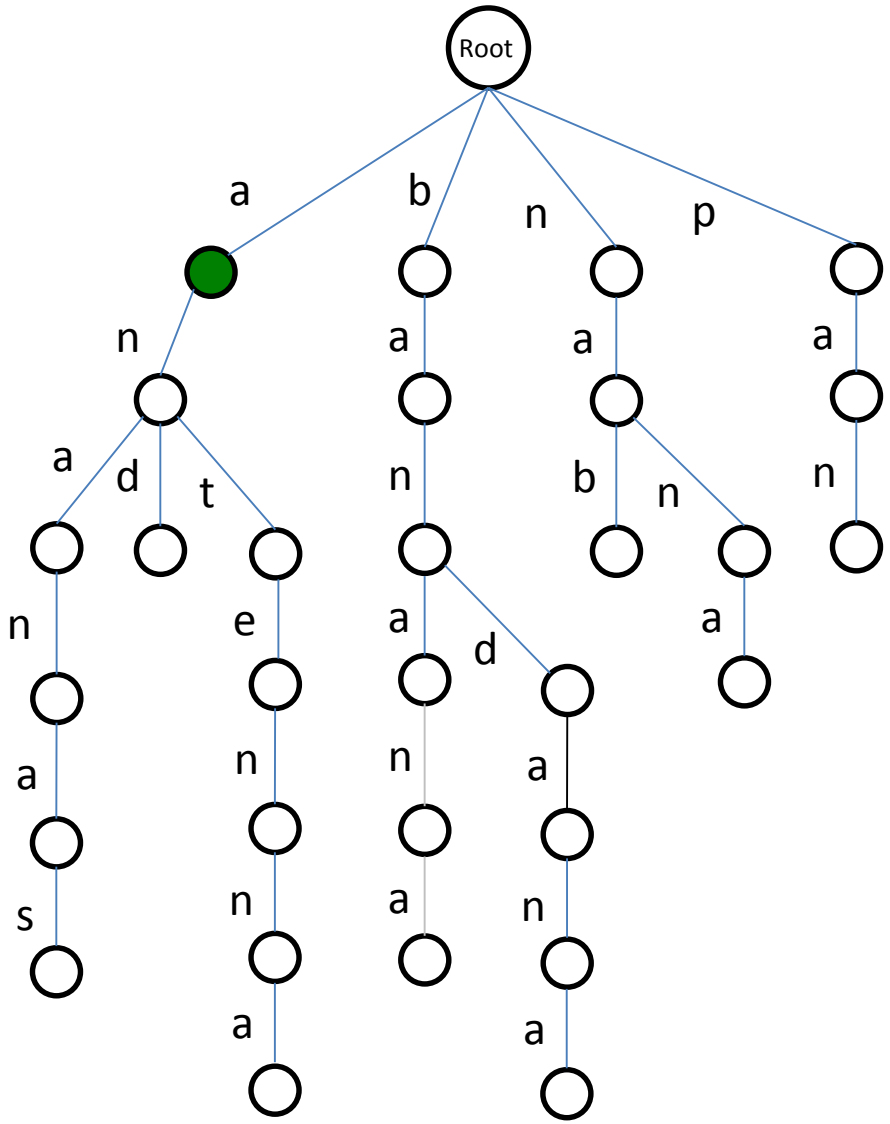
p a n a m a b a n a n a s



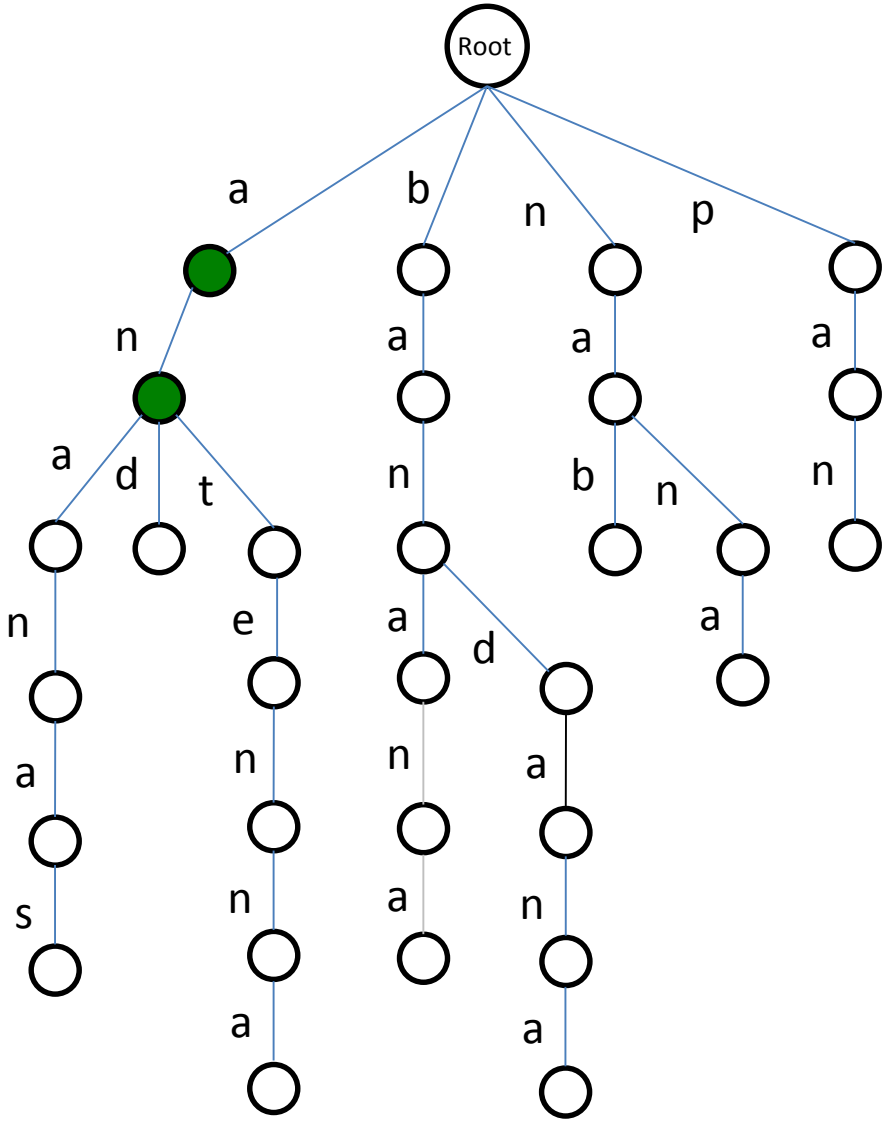
p a n a m a b a n a n a s



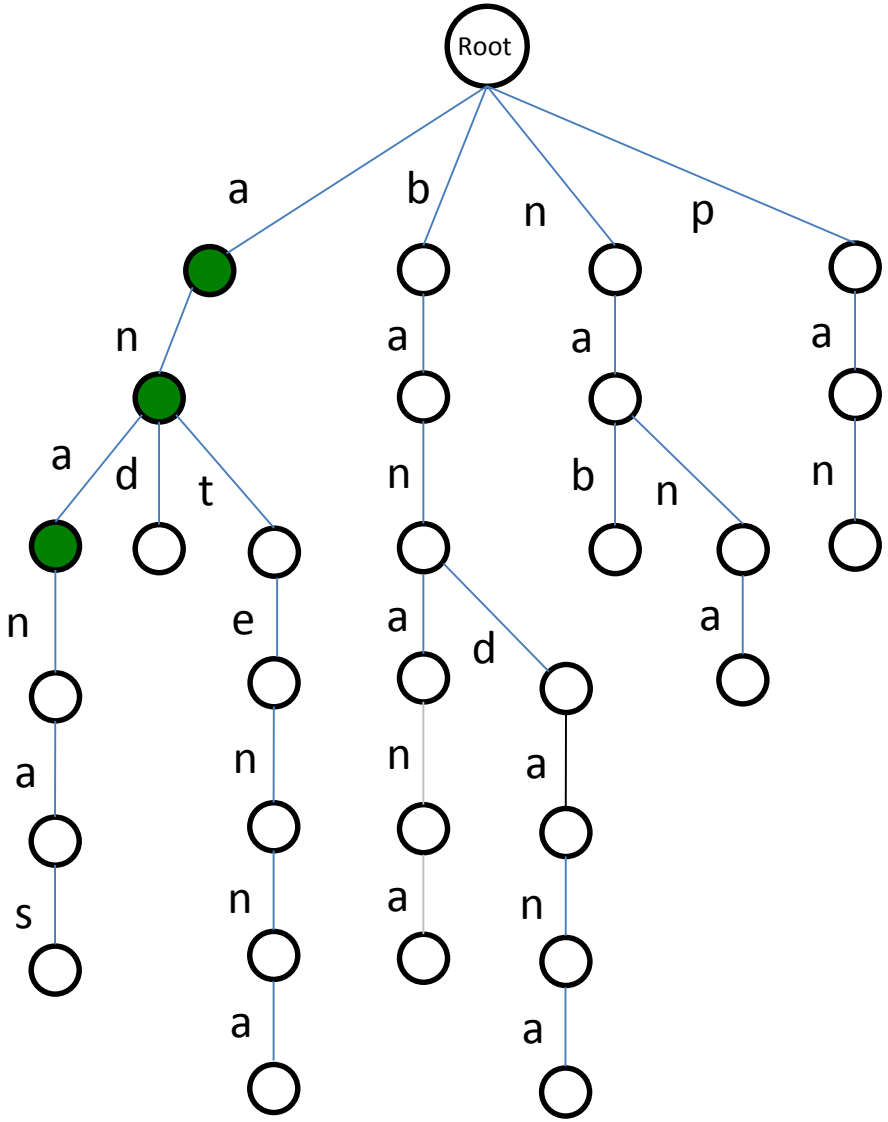
p a n a m a b a n a n a s



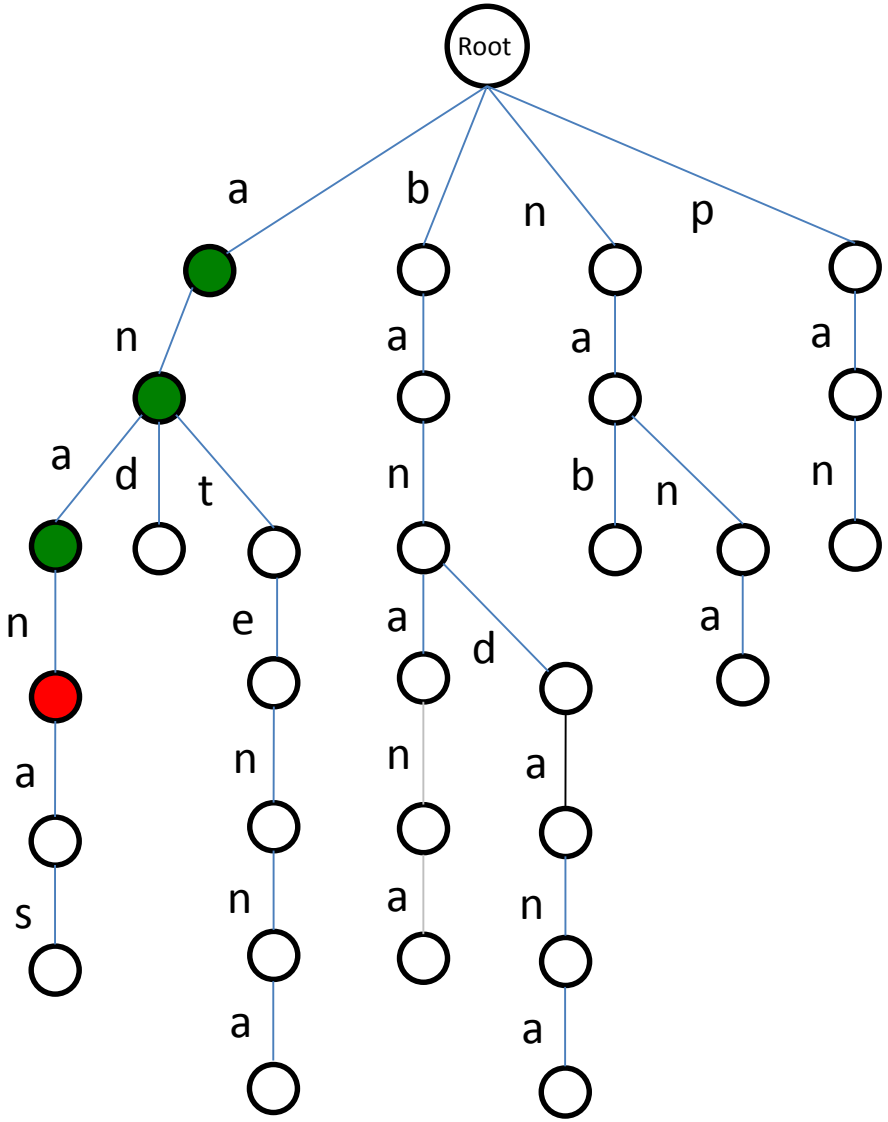
p a n a m a b a n a n a s



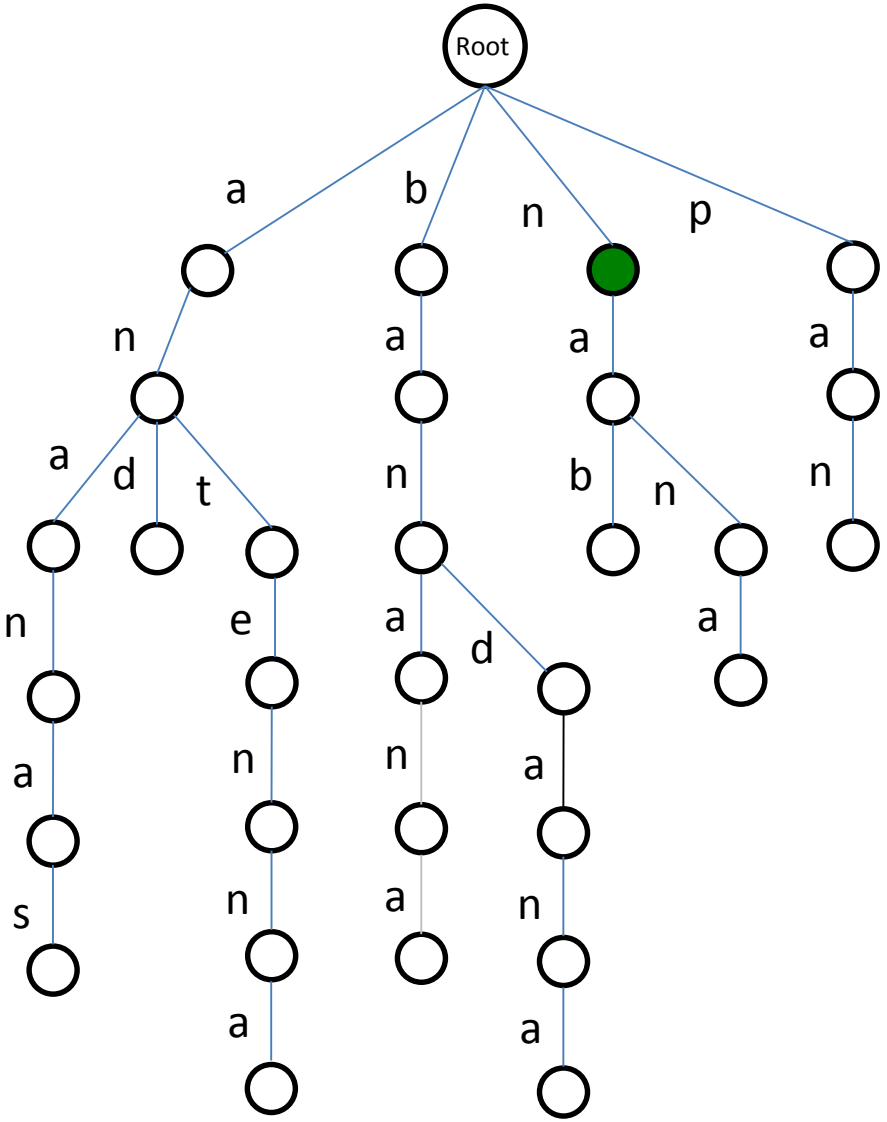
p a n a m a b a n a n a s



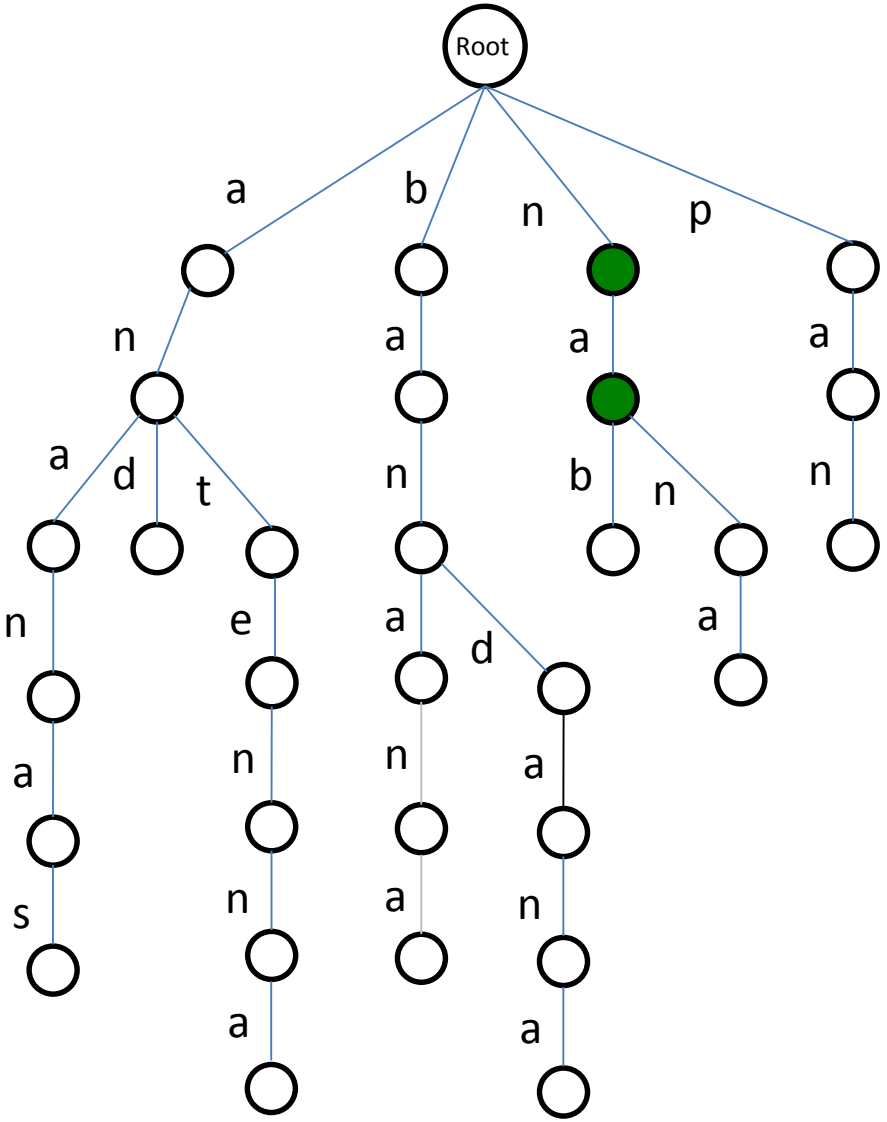
p a n a m a b a n a n a s



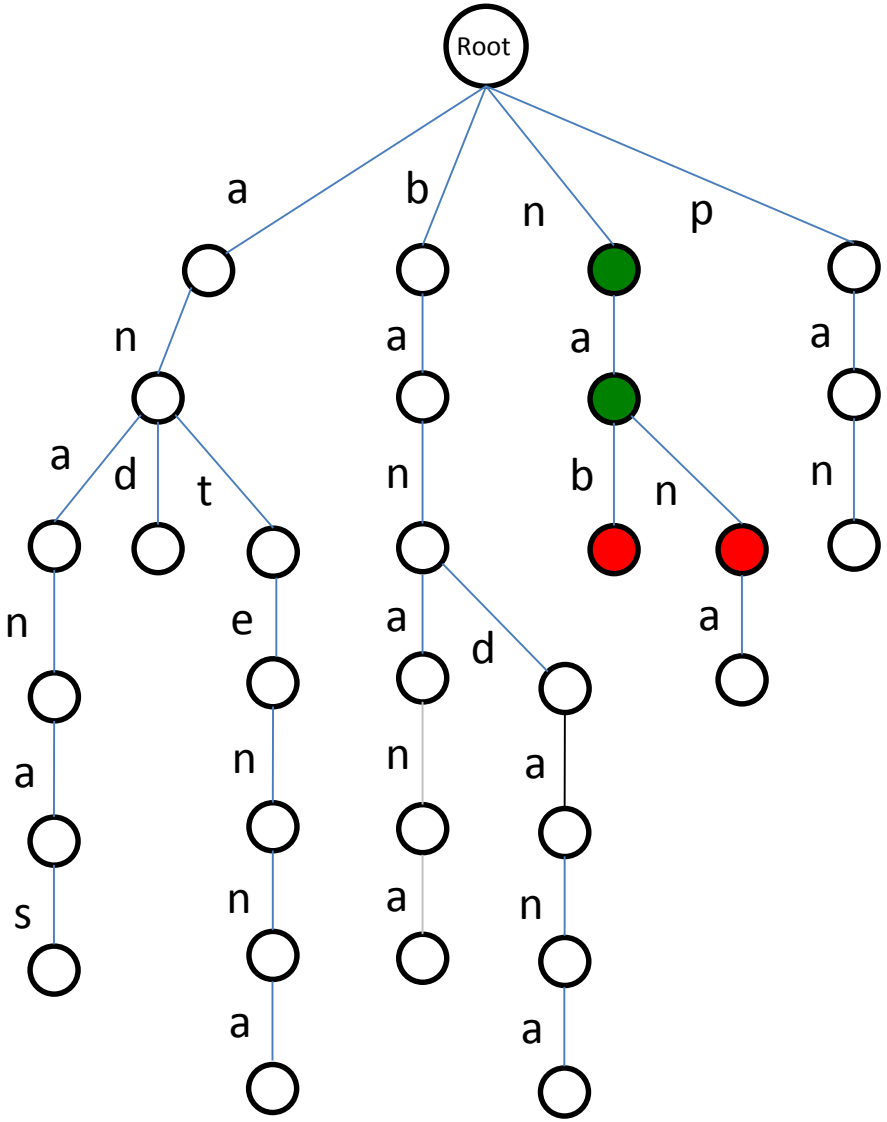
p a n a m a b a n a n a s



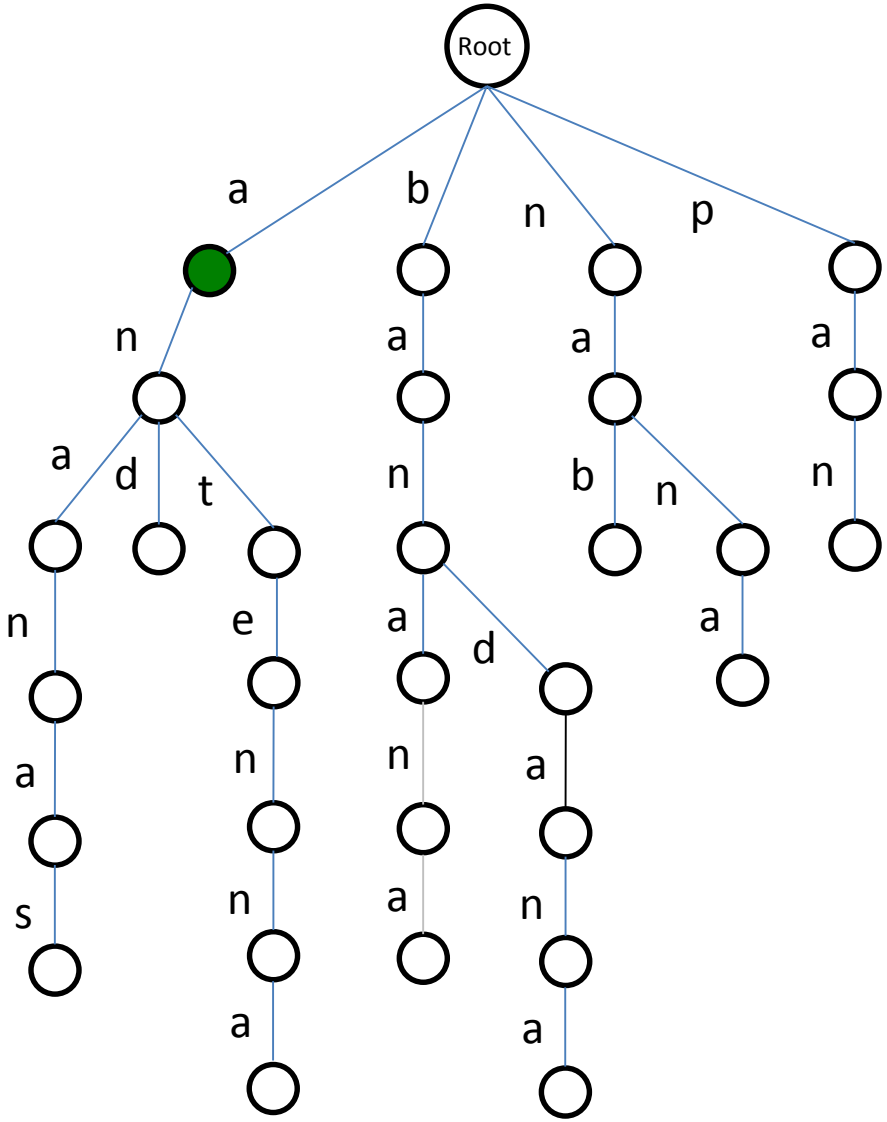
p a n a m a b a n a n a s



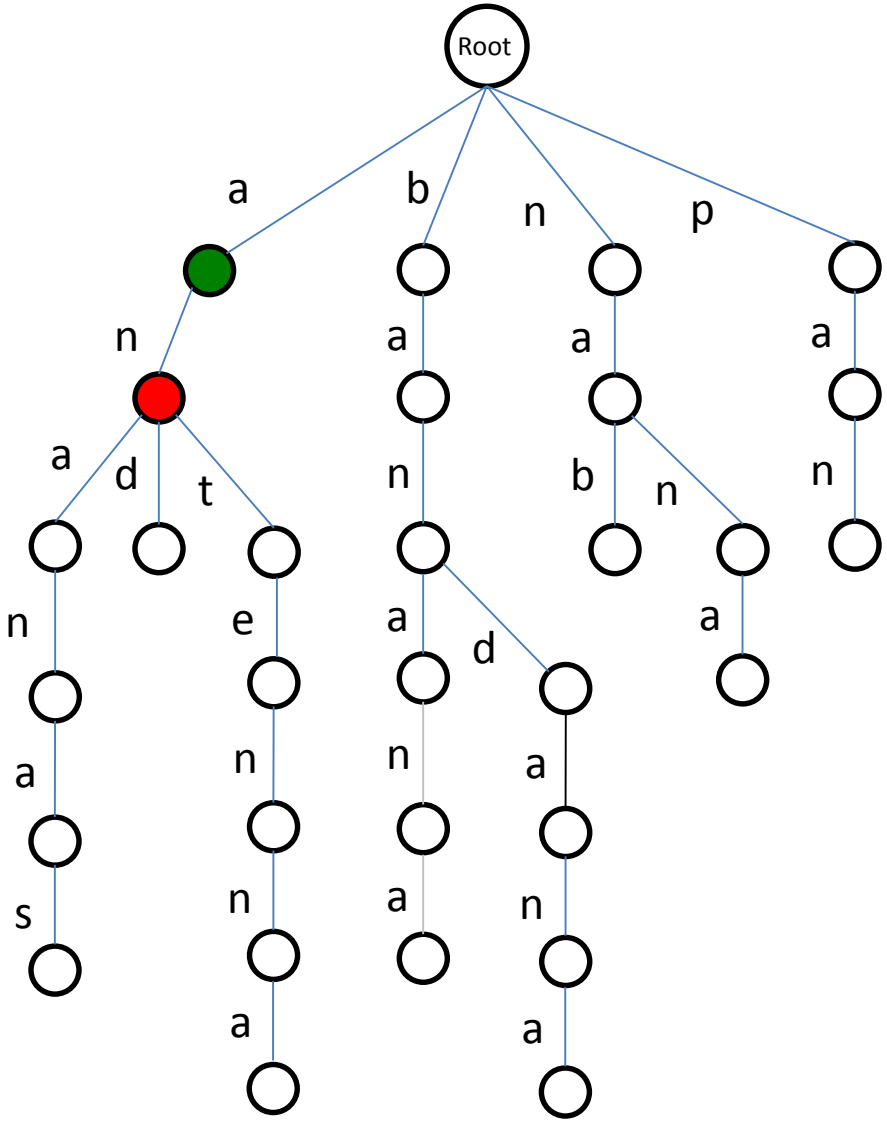
p a n a m a b a n a n a s



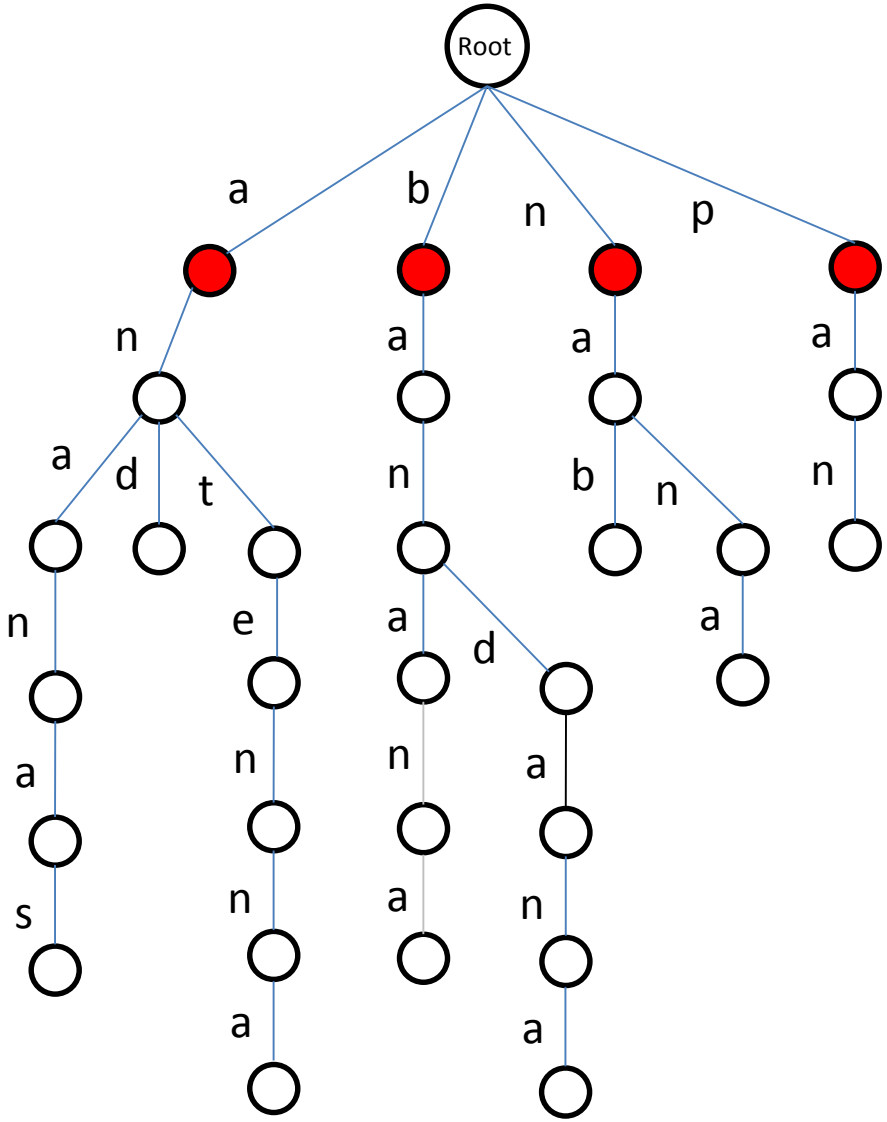
p a n a m a b a n a n a s



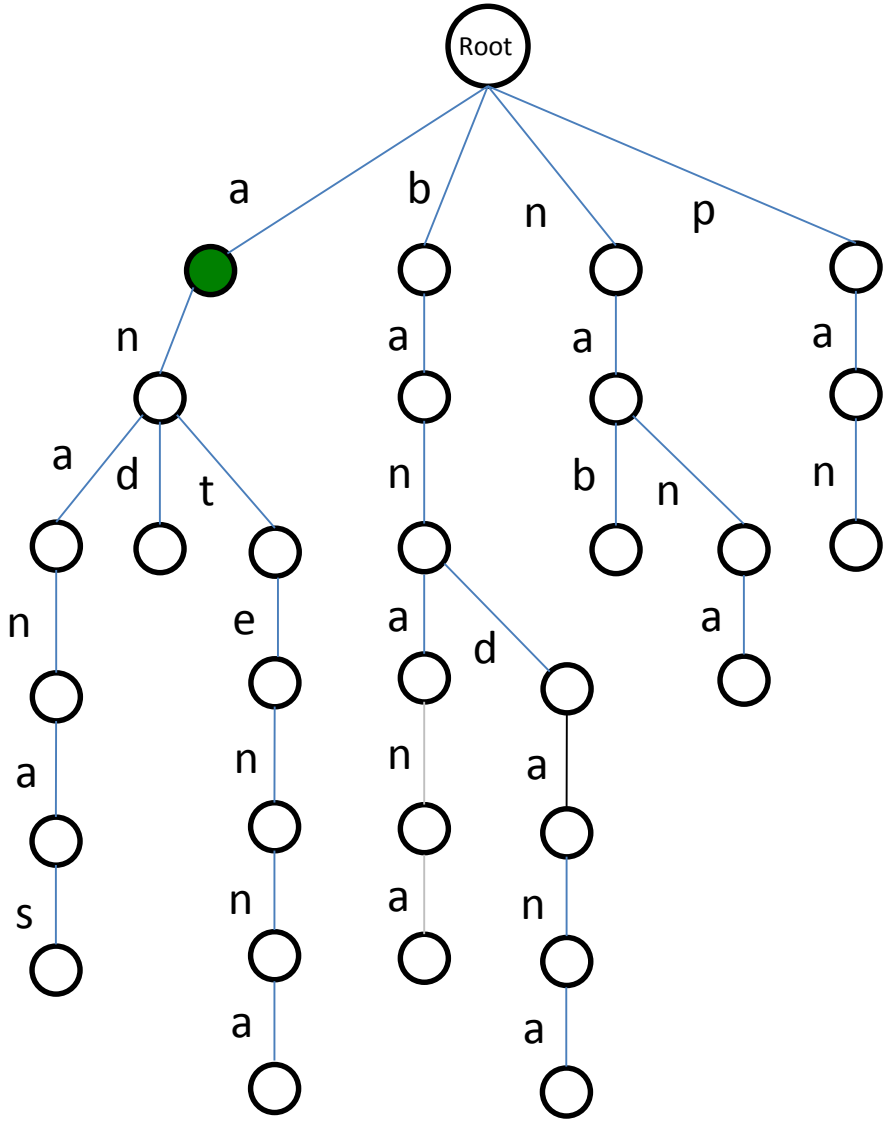
p a n a m a b a n a n a s



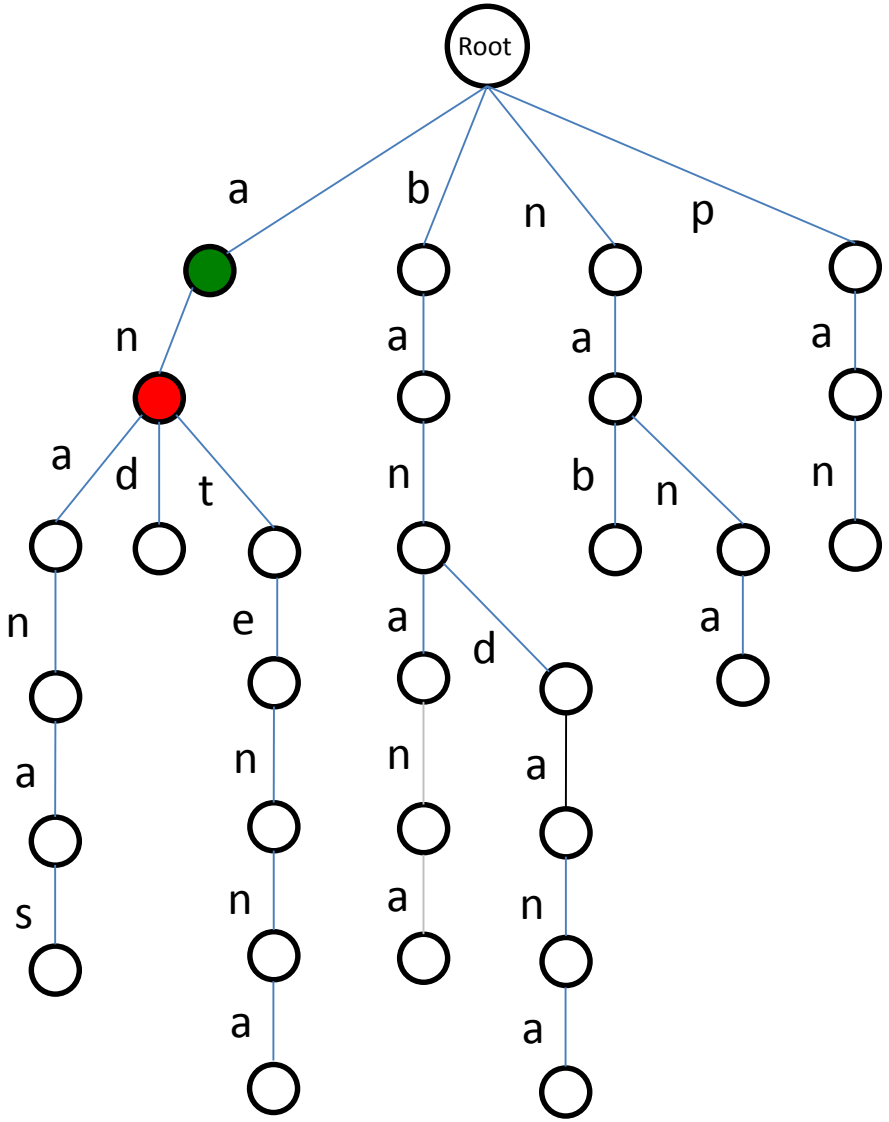
p a n a m a b a n a n a s



p a n a m **a** b a n a n a s



p a n a m a b a n a n a s



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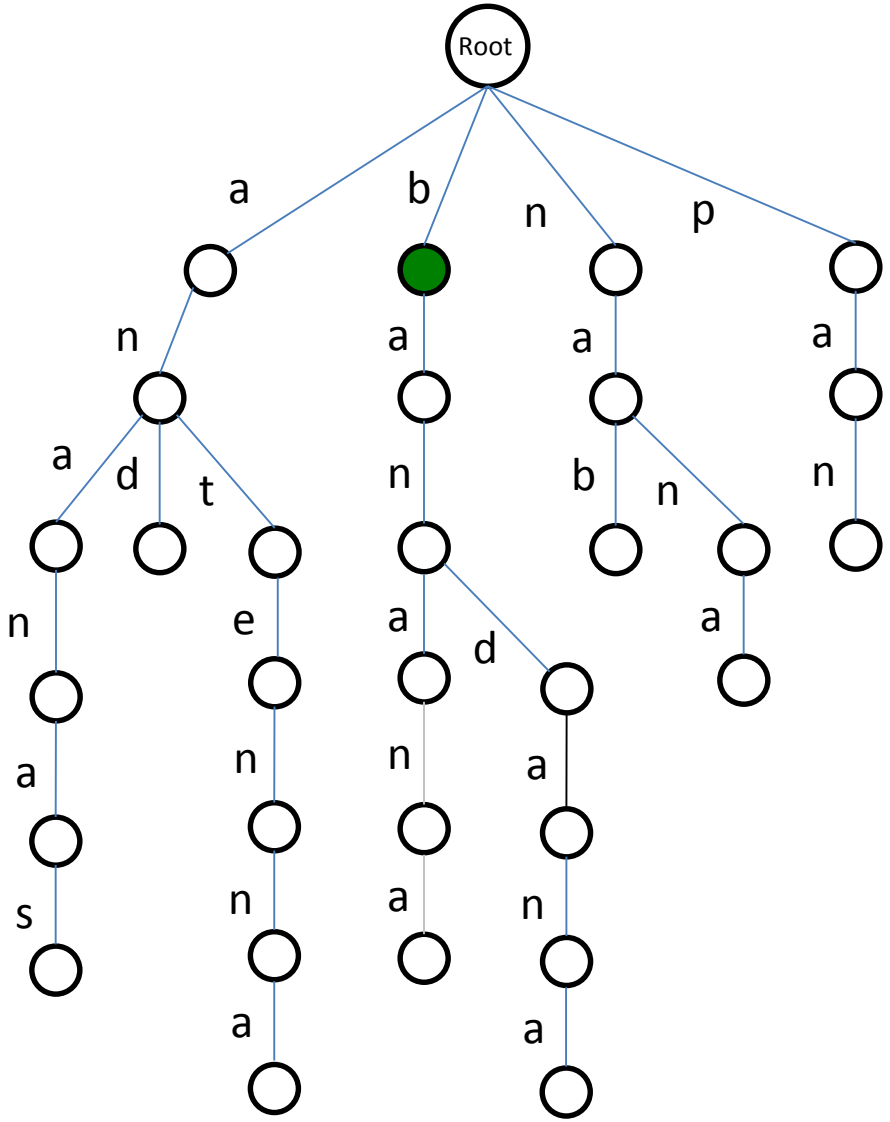

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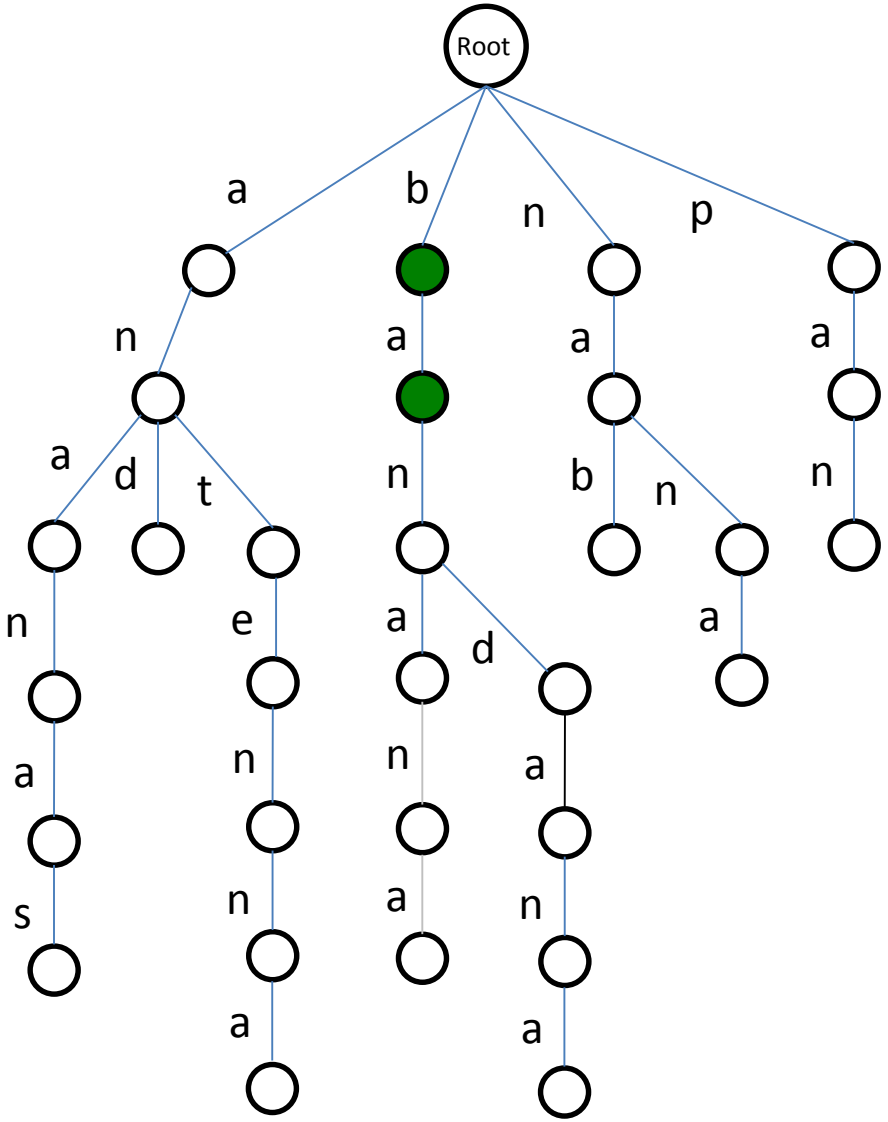

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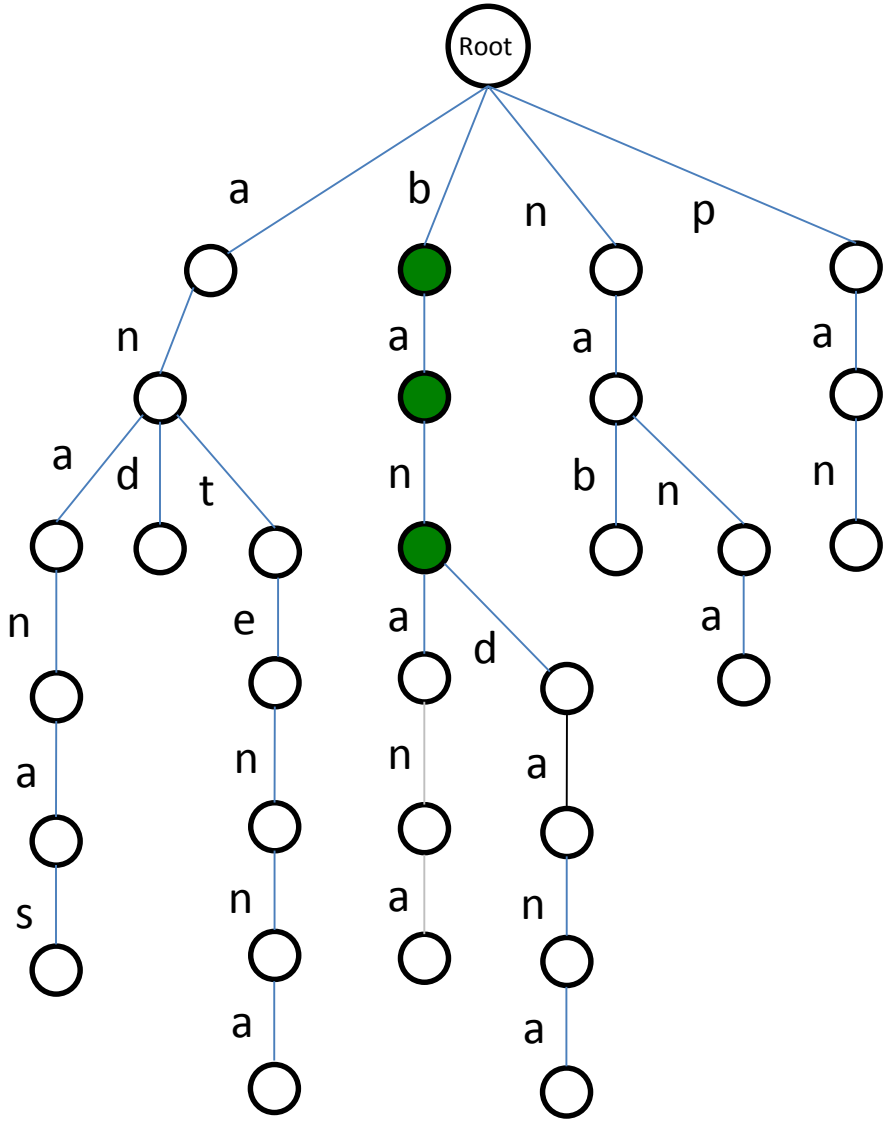

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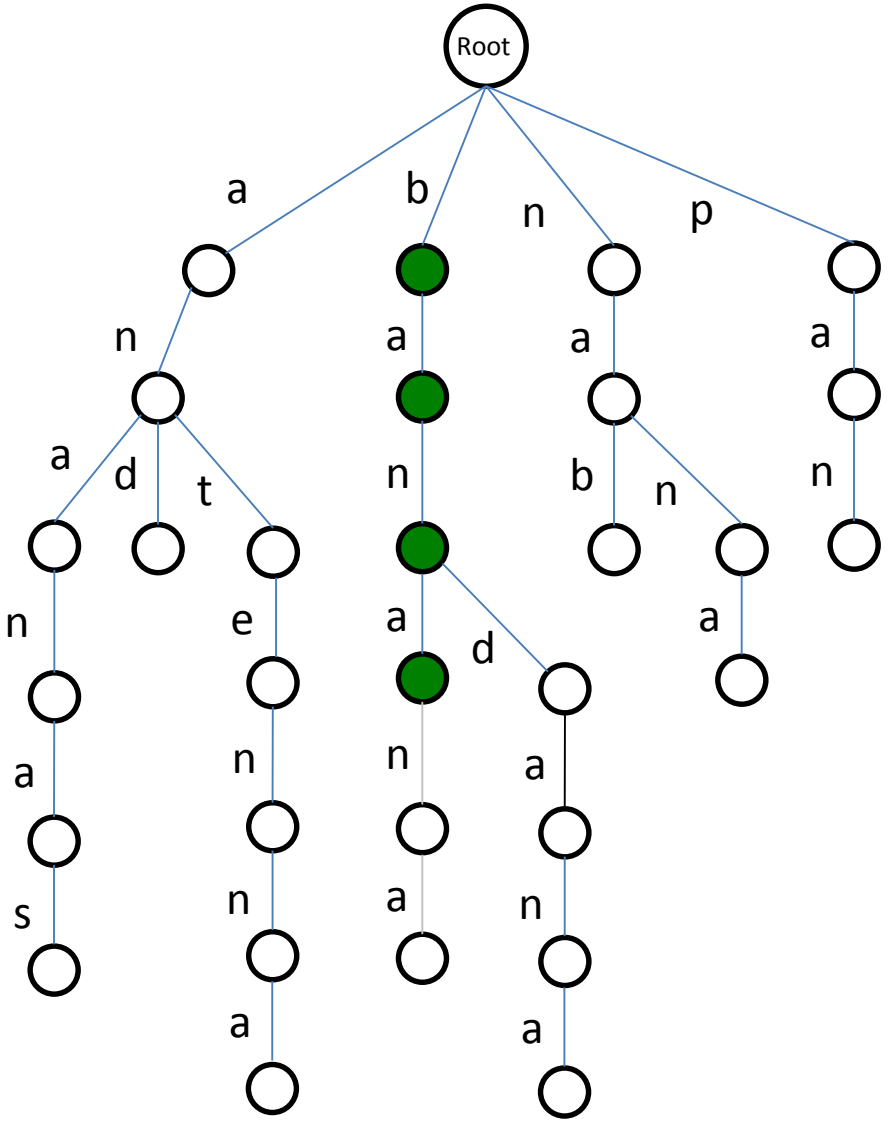

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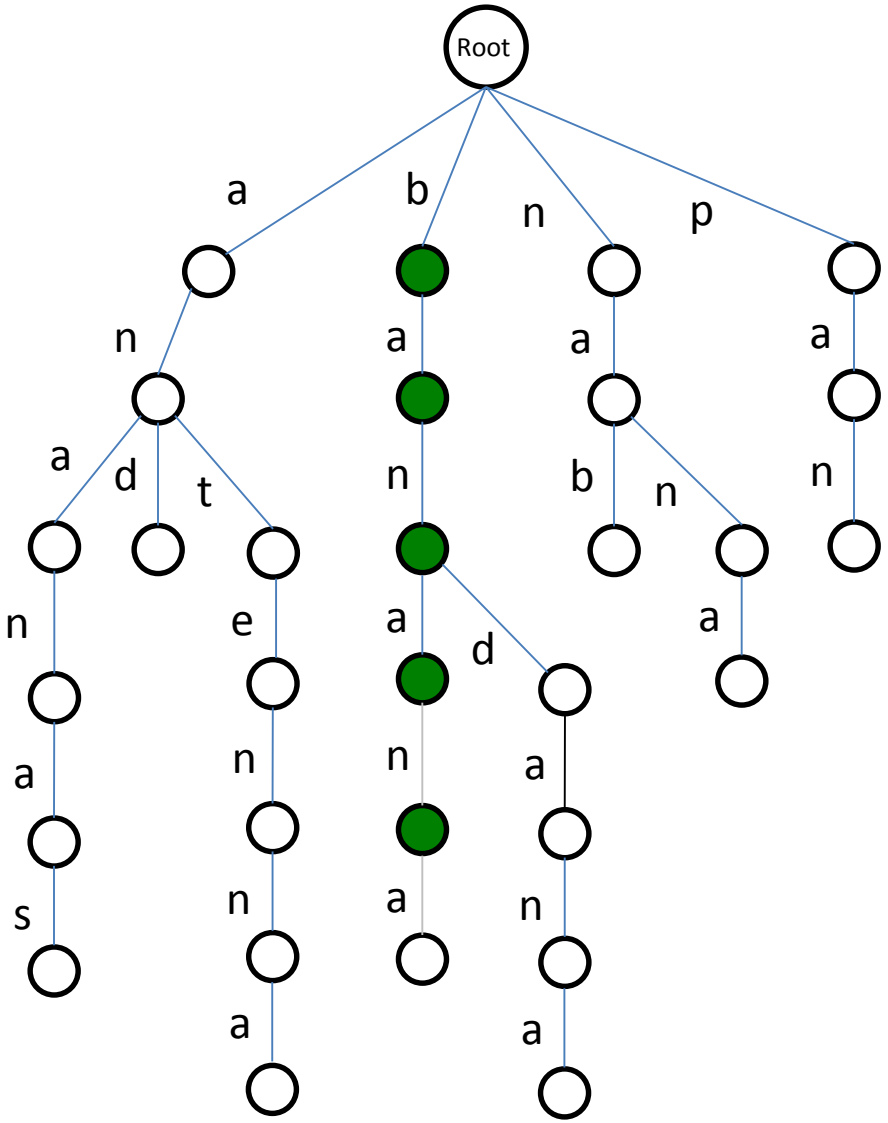

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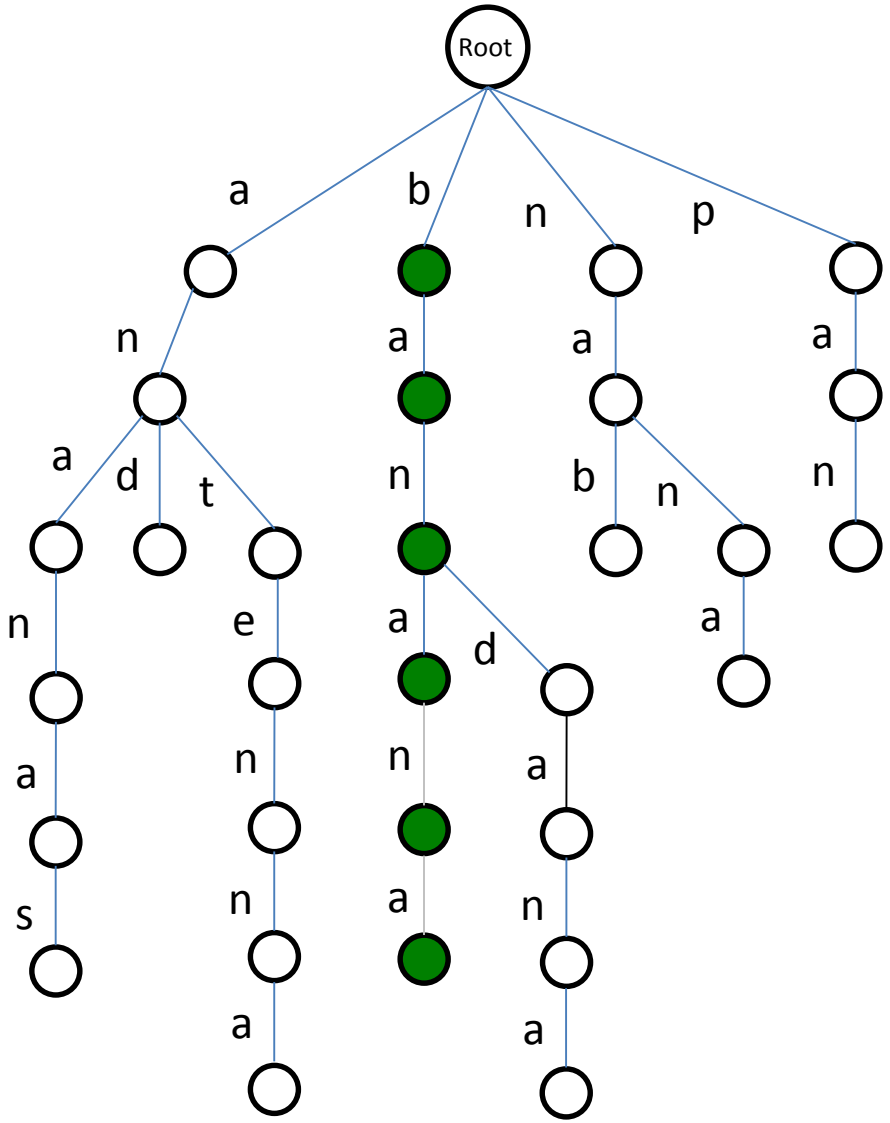
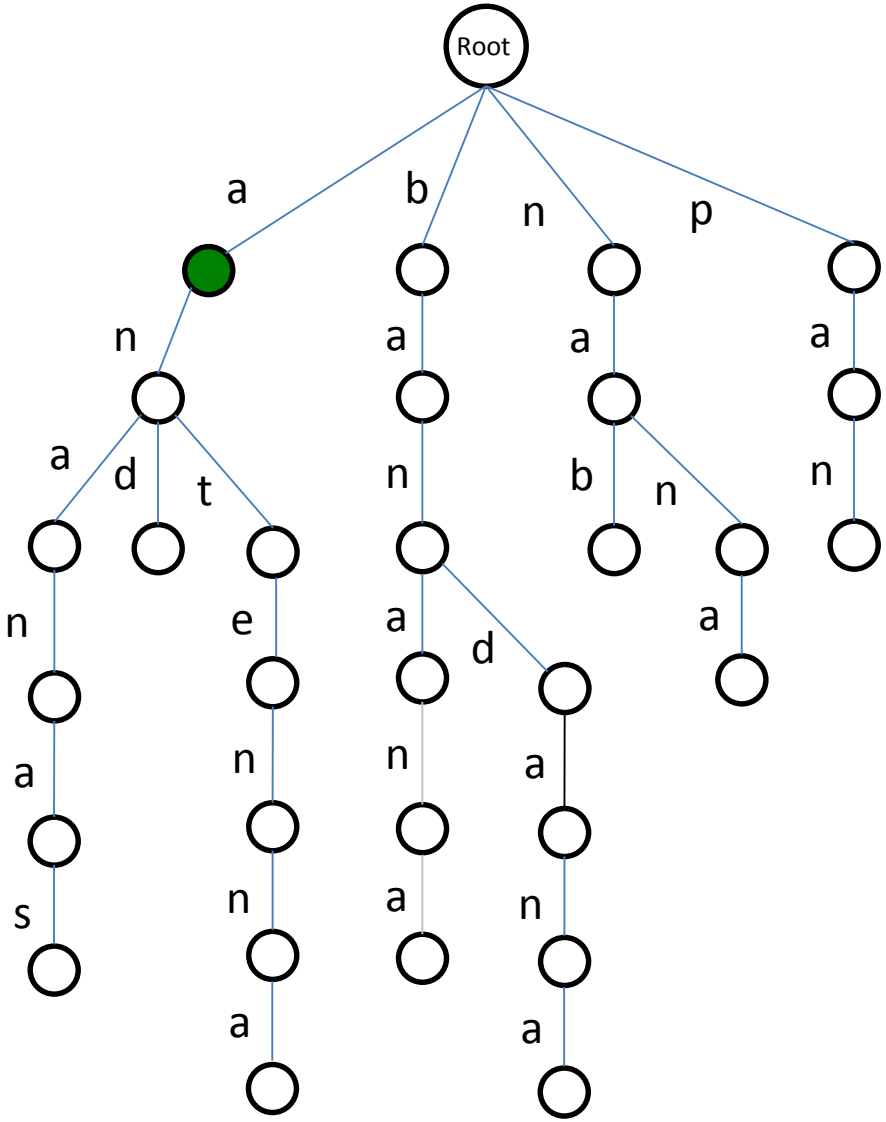


p a n a m a b a n a n a s



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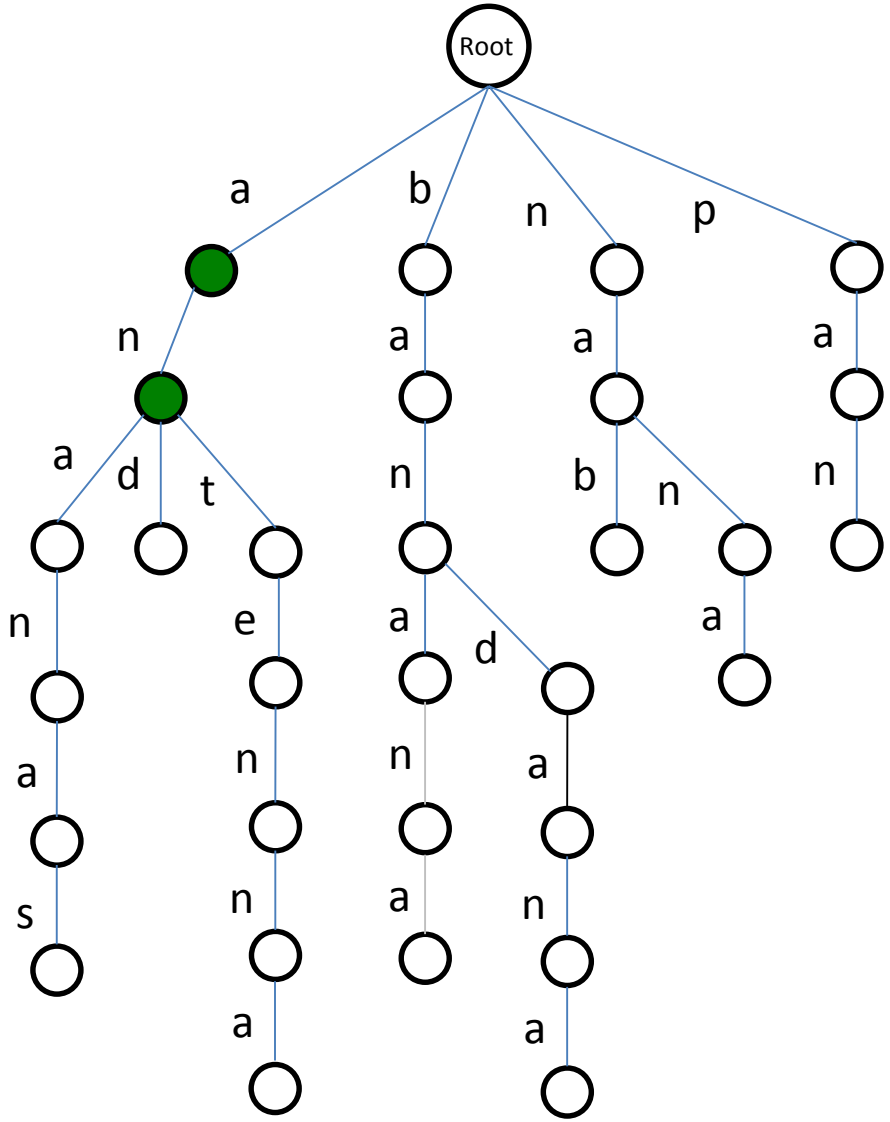

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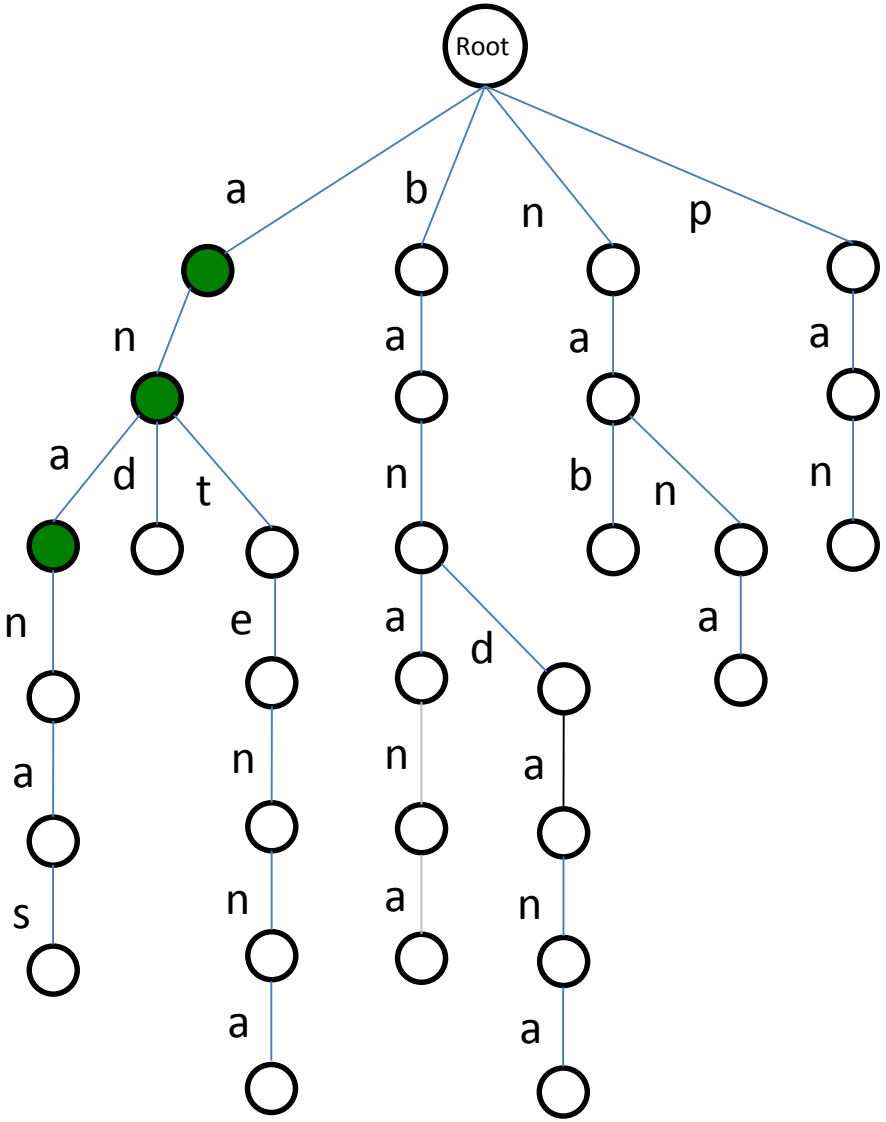
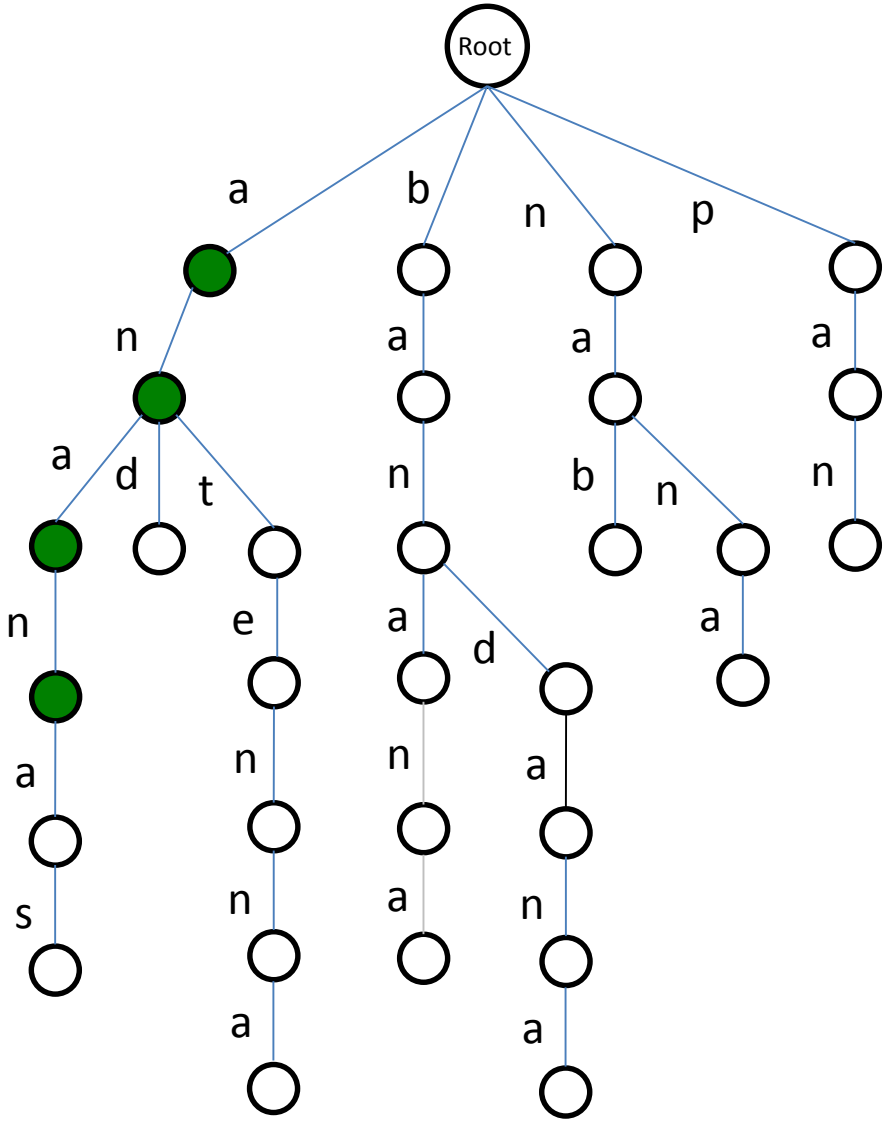


p a n a m a b **a n a n** a s



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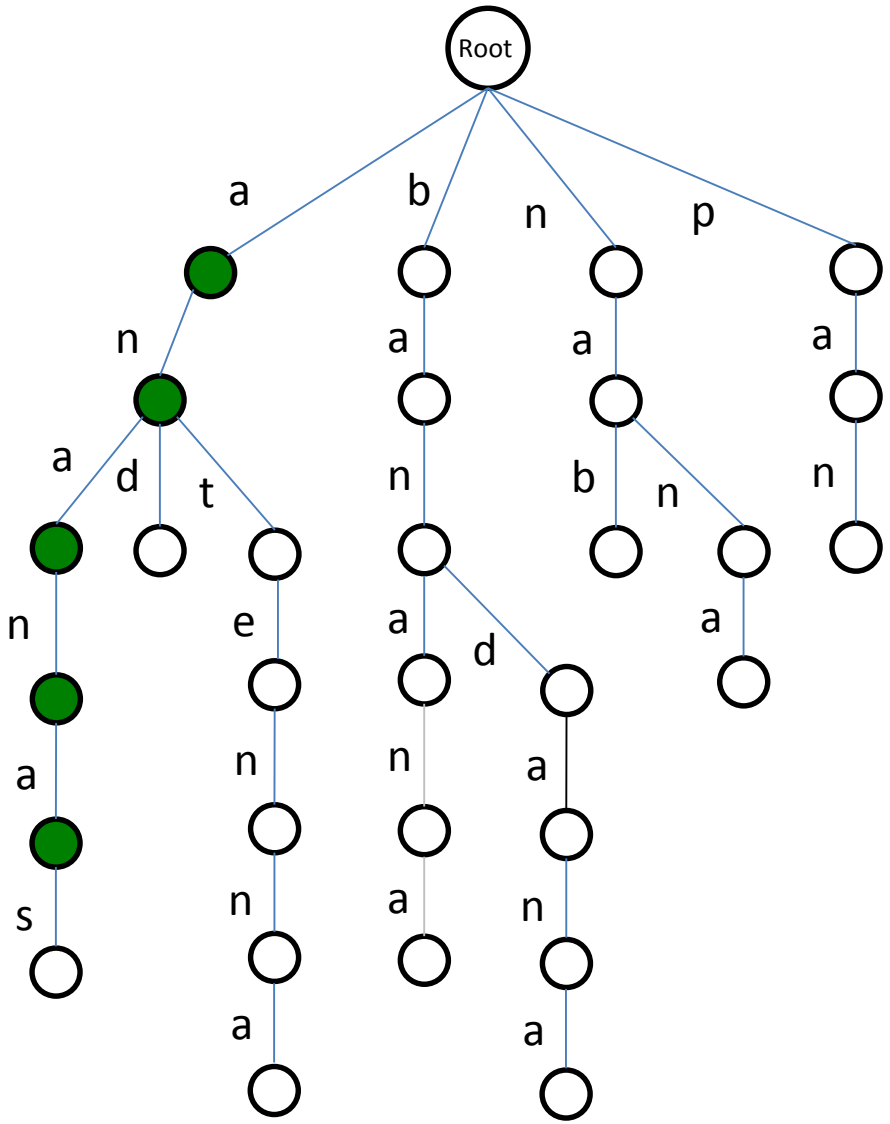

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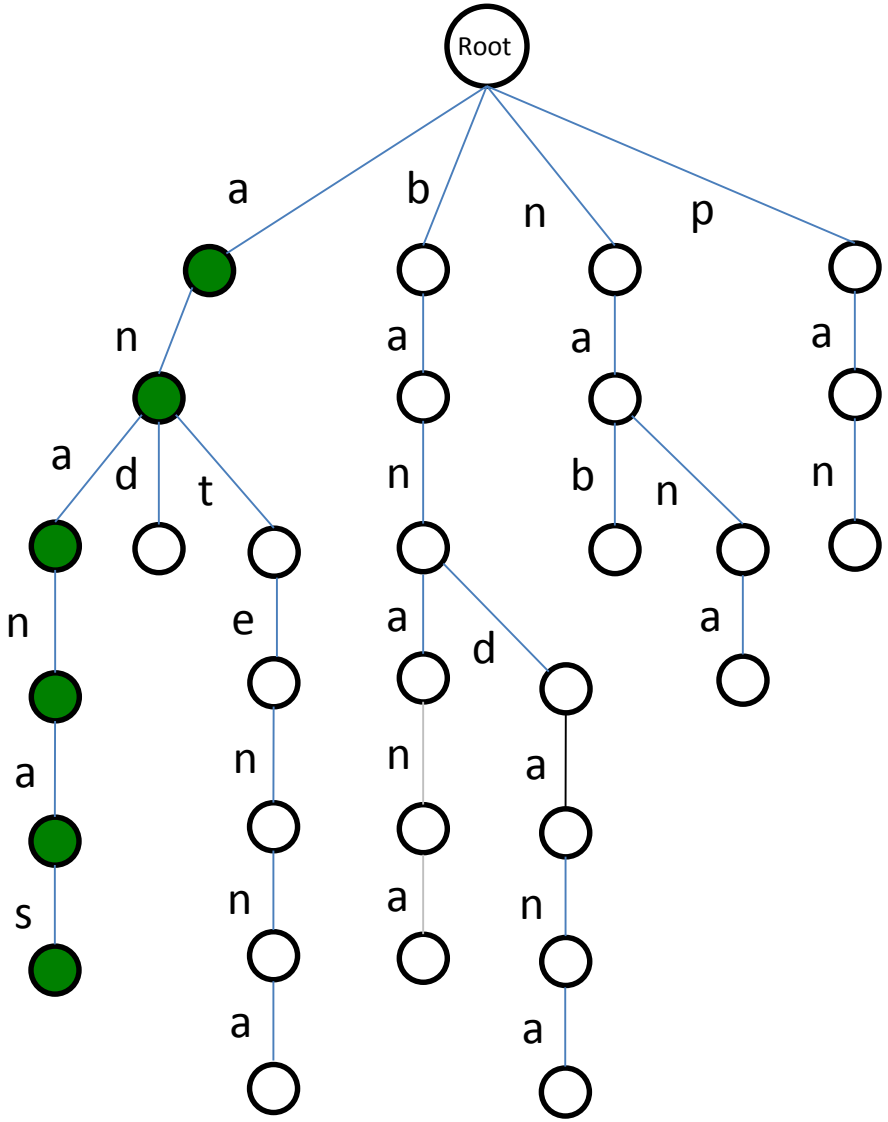
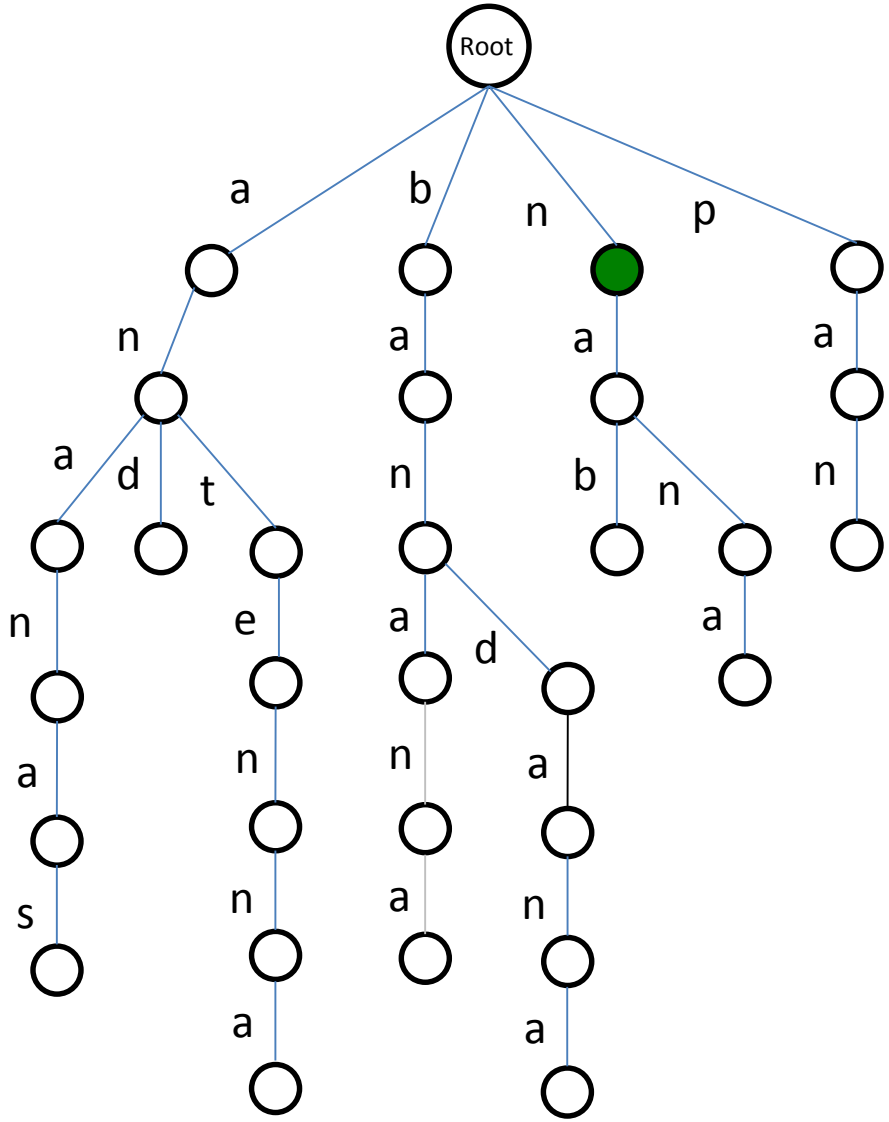
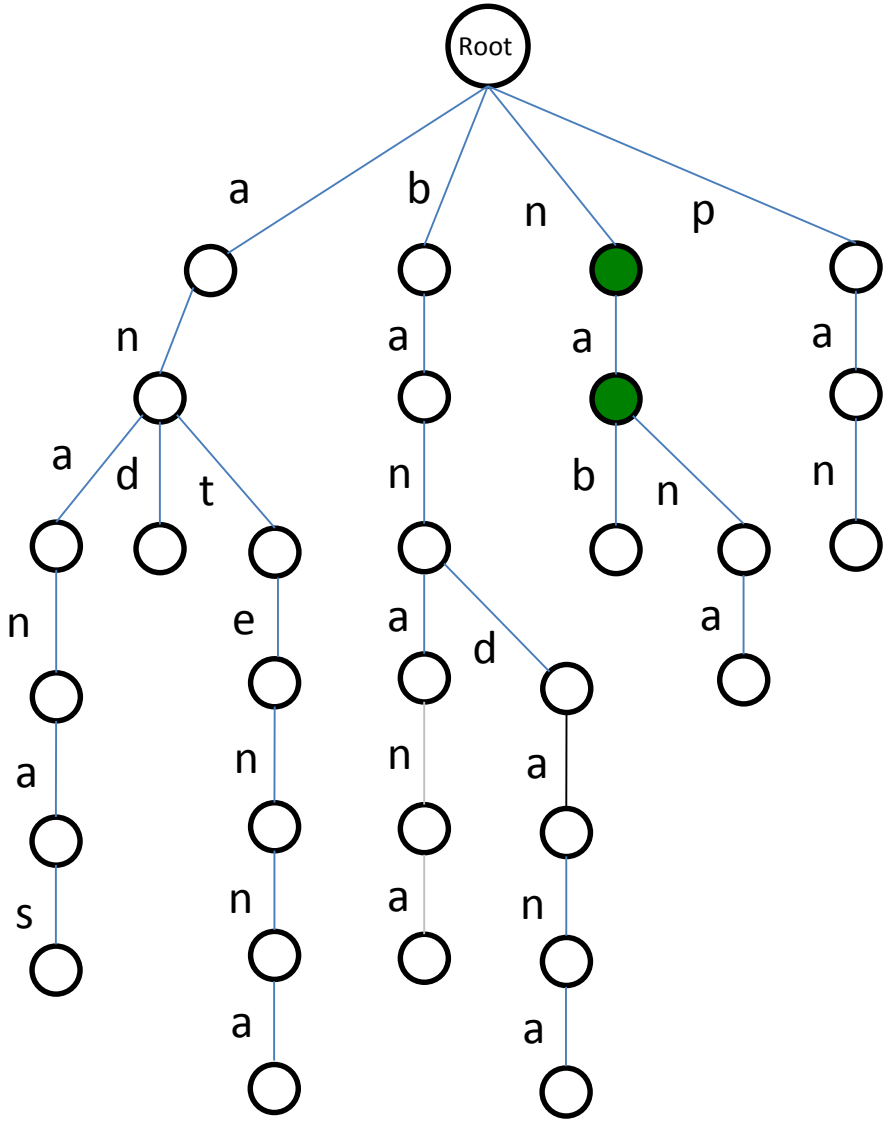


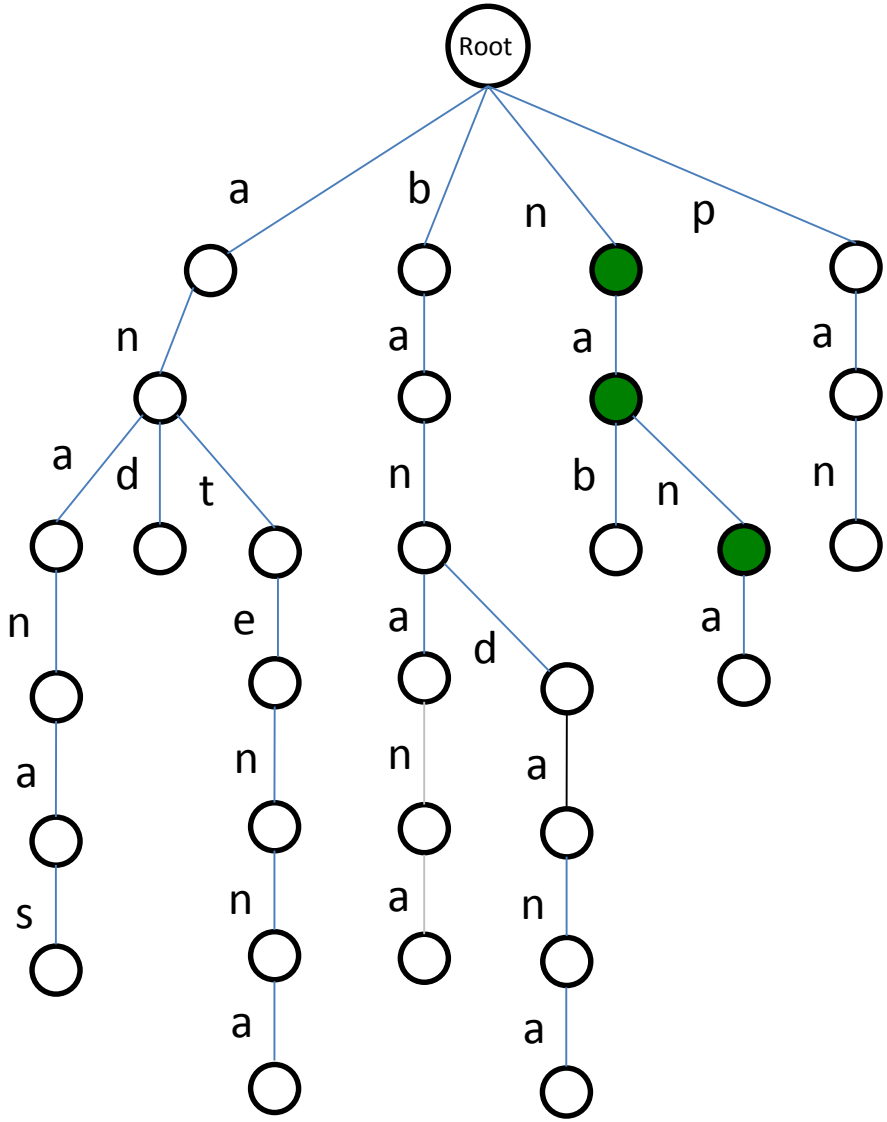
p a n a m a b a **n** a n a s



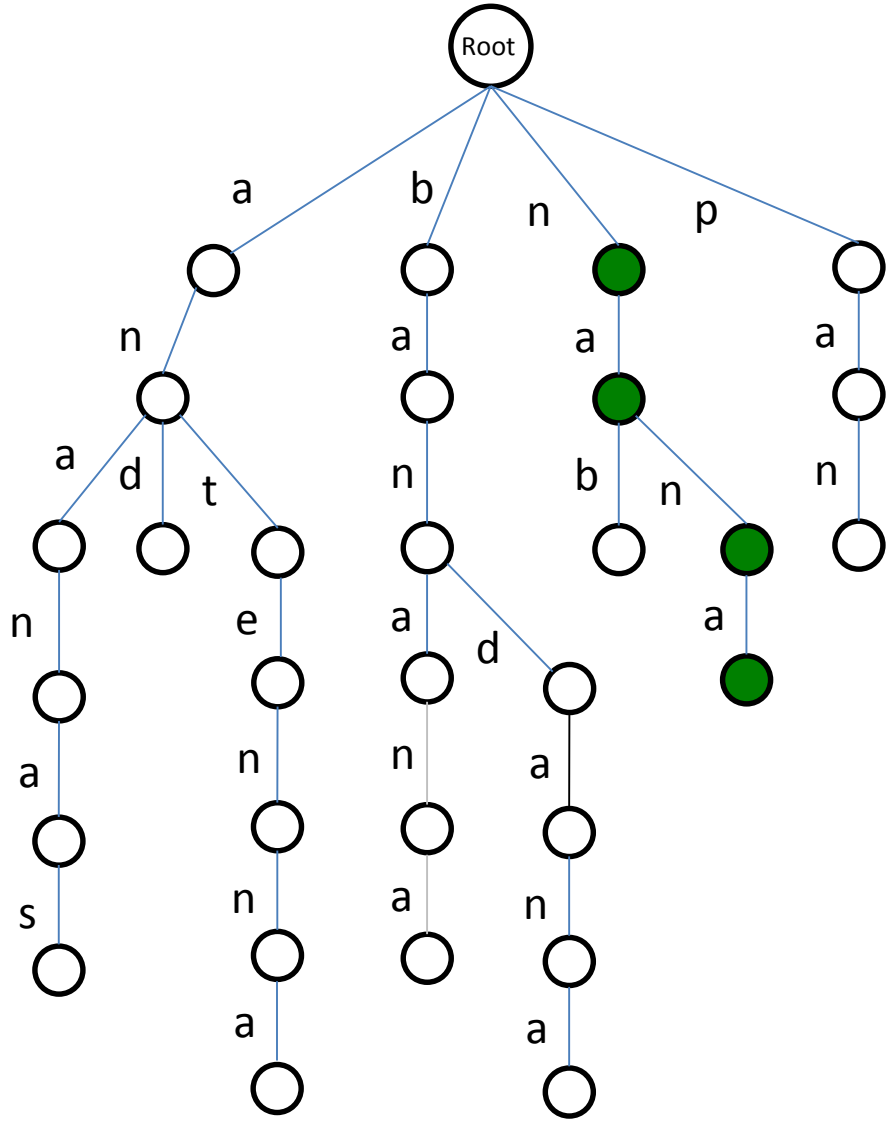
p a n a m a b a **n a** n a s



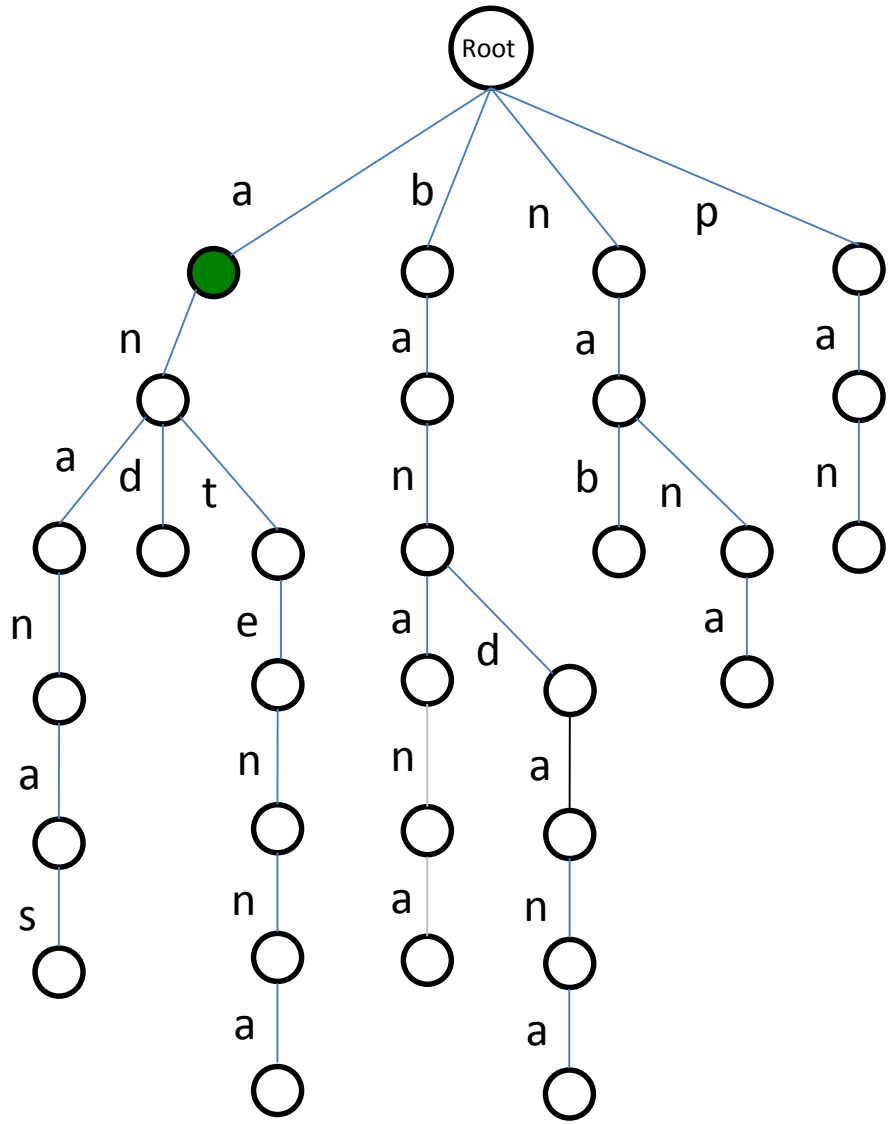
p a n a m a b a **n a n** a s



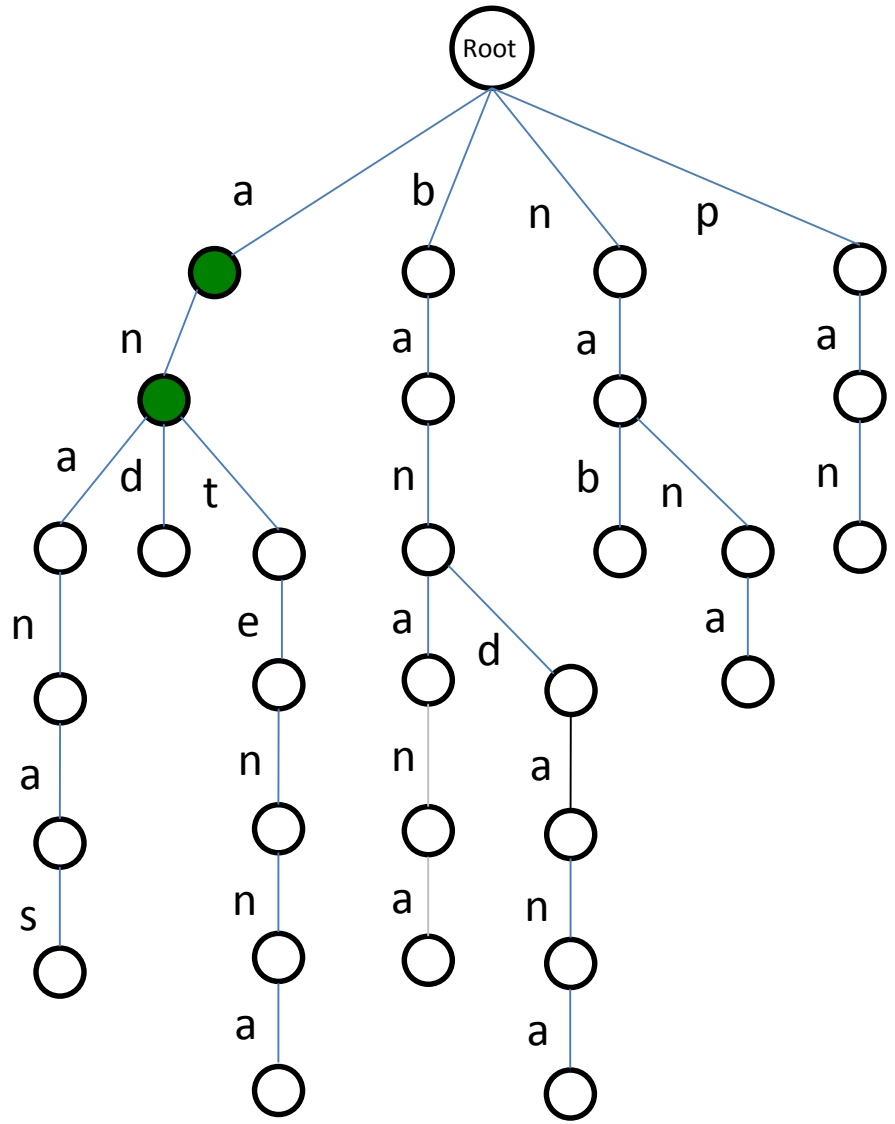
p a n a m a b a **n a n a** s



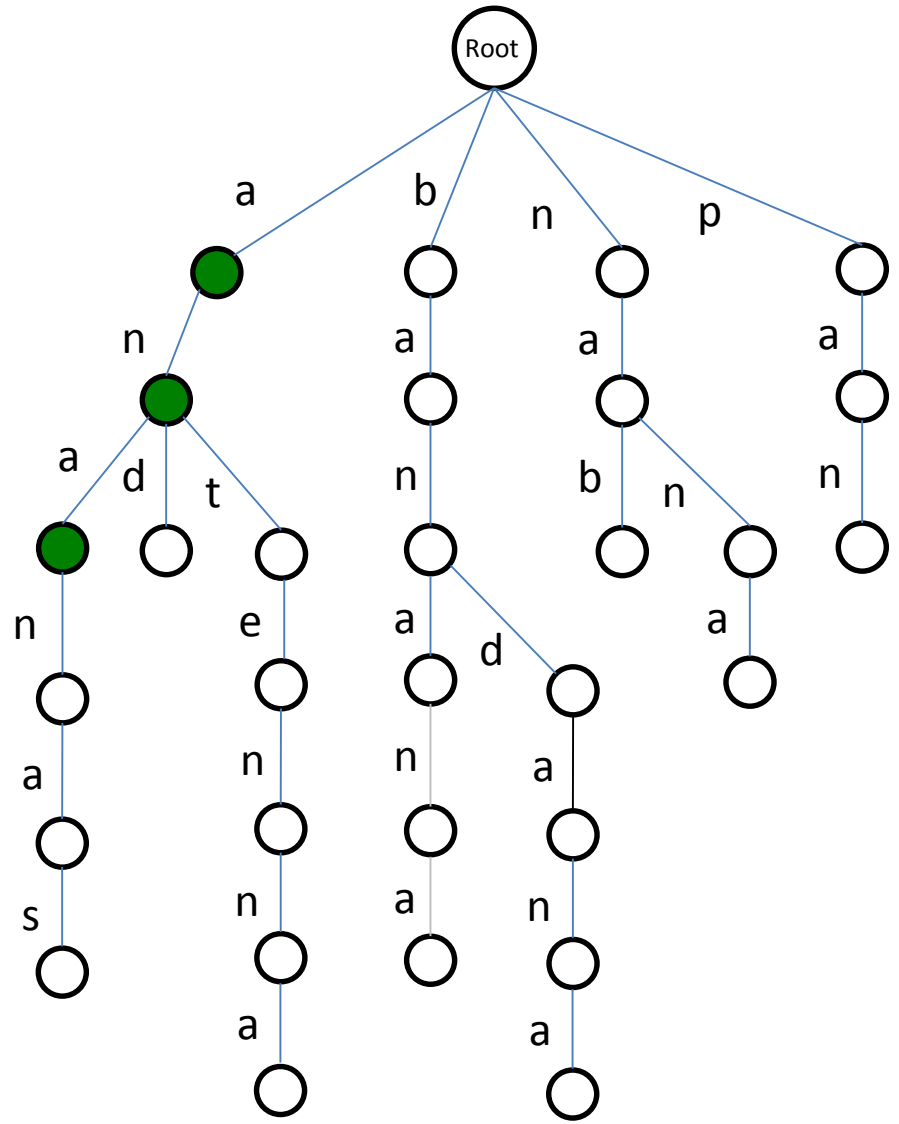
p a n a m a b a n **a** n a s



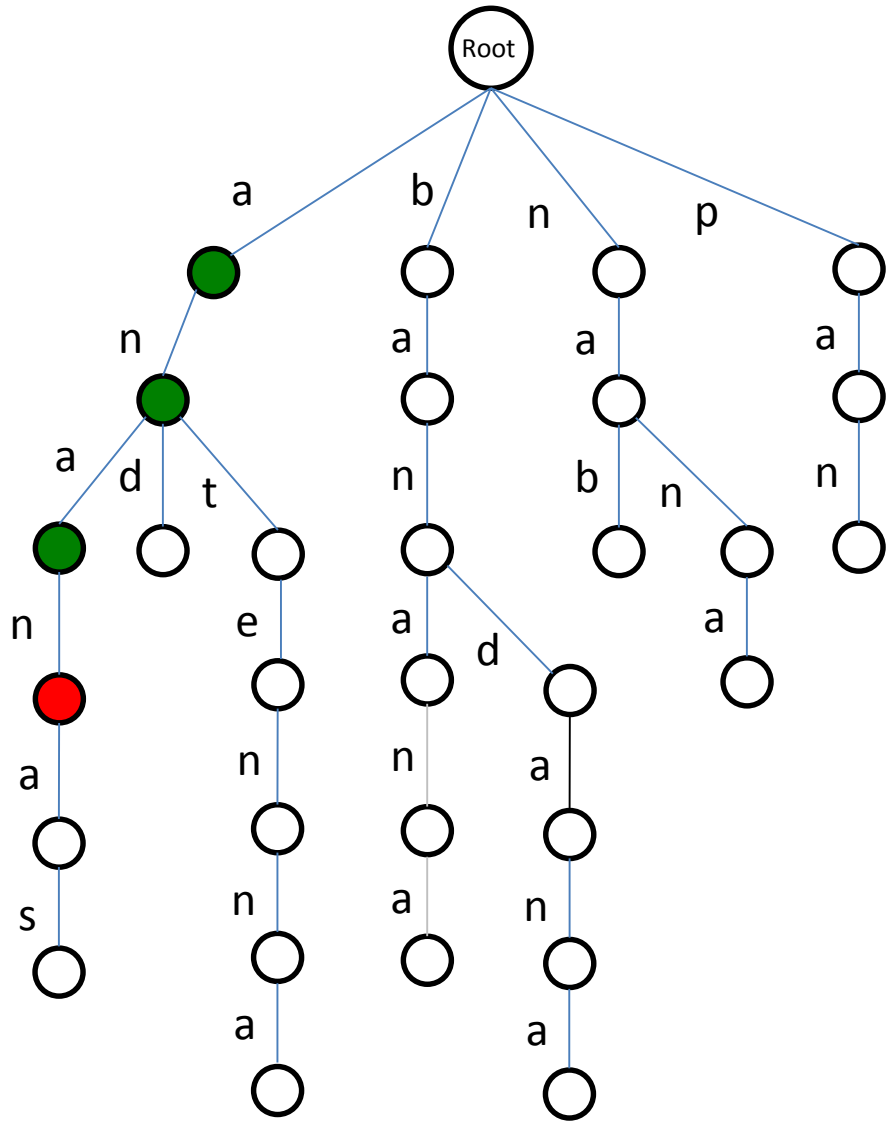
p a n a m a b a n **a n** a s



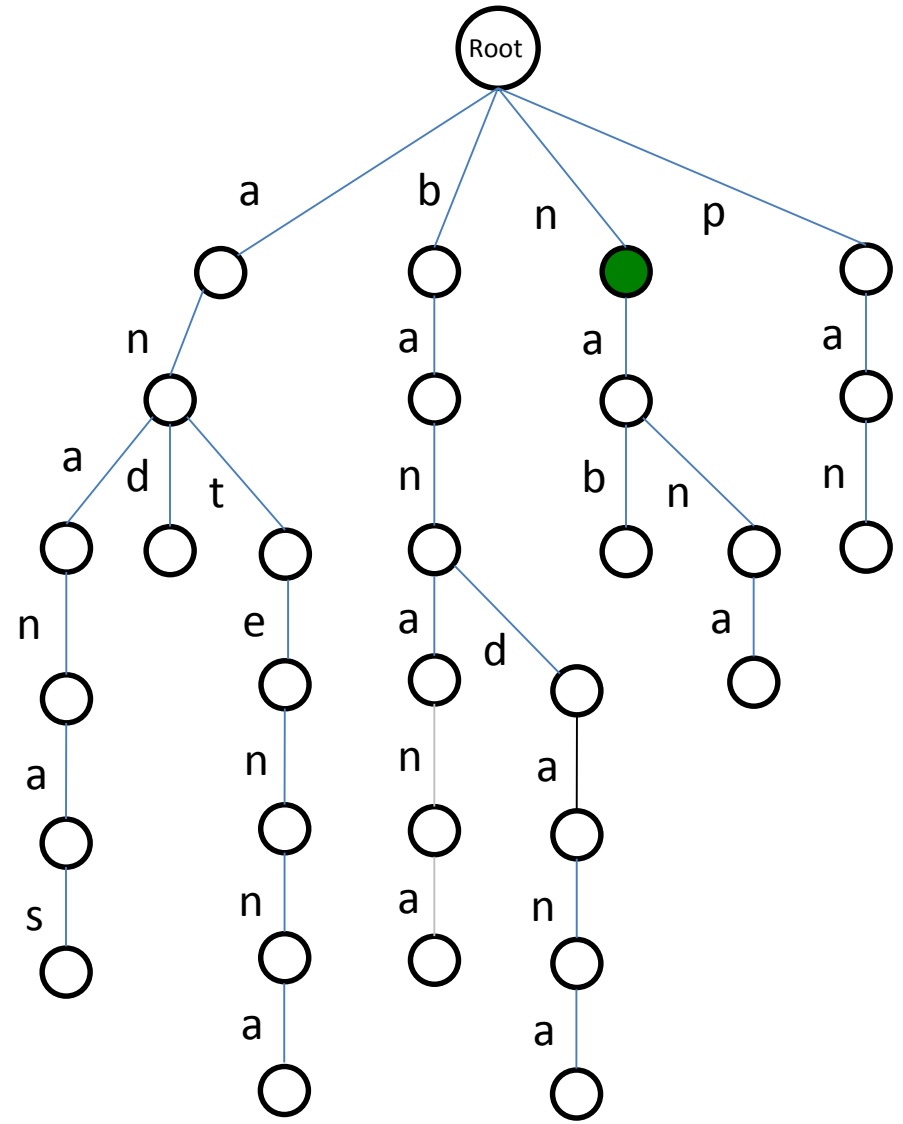
p a n a m a b a n **a n a** s



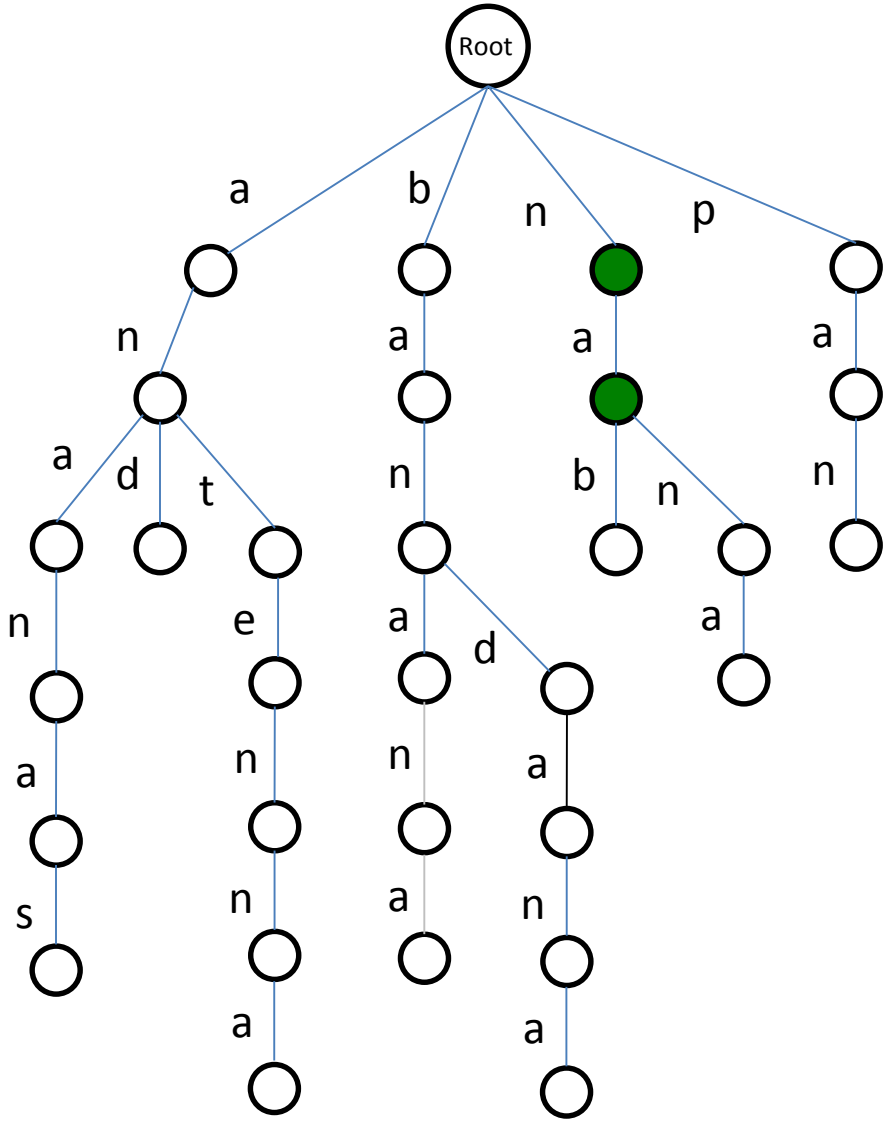
p a n a m a b a n **a n a s**



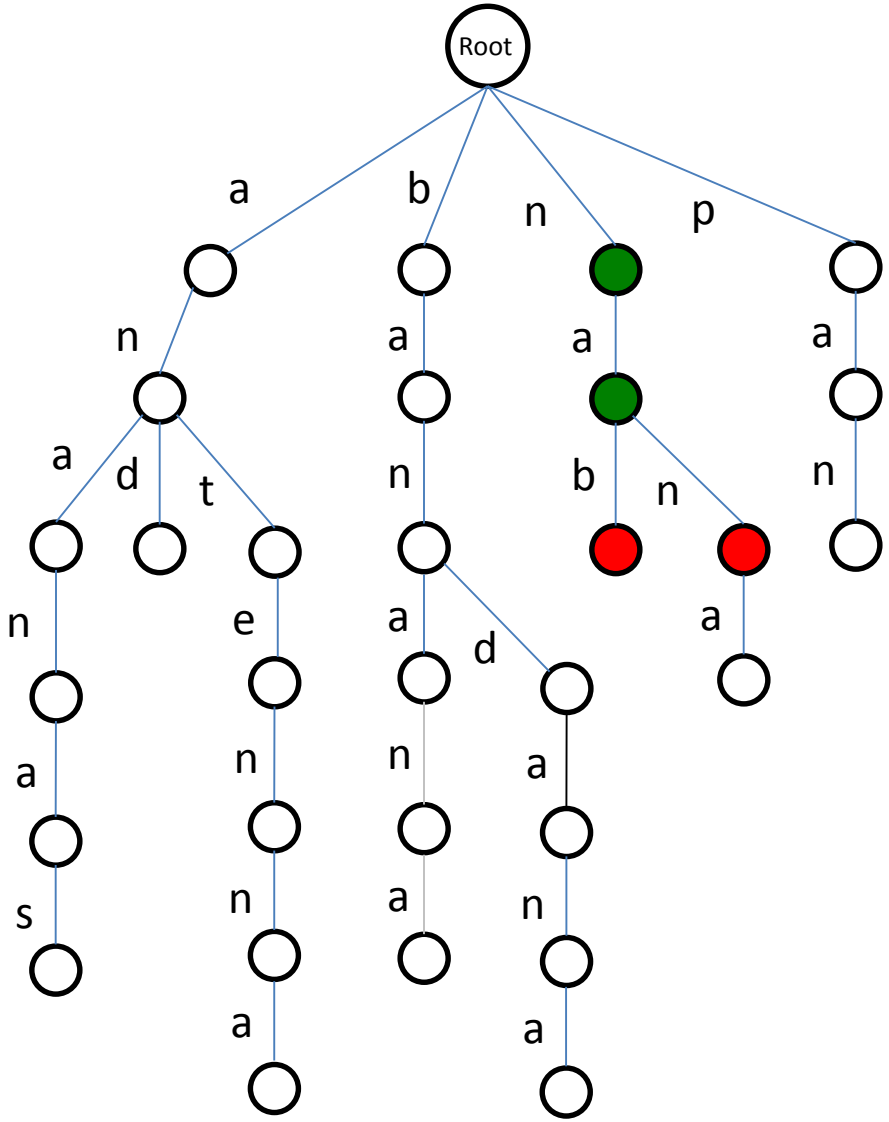
p a n a m a b a n a **n** a s



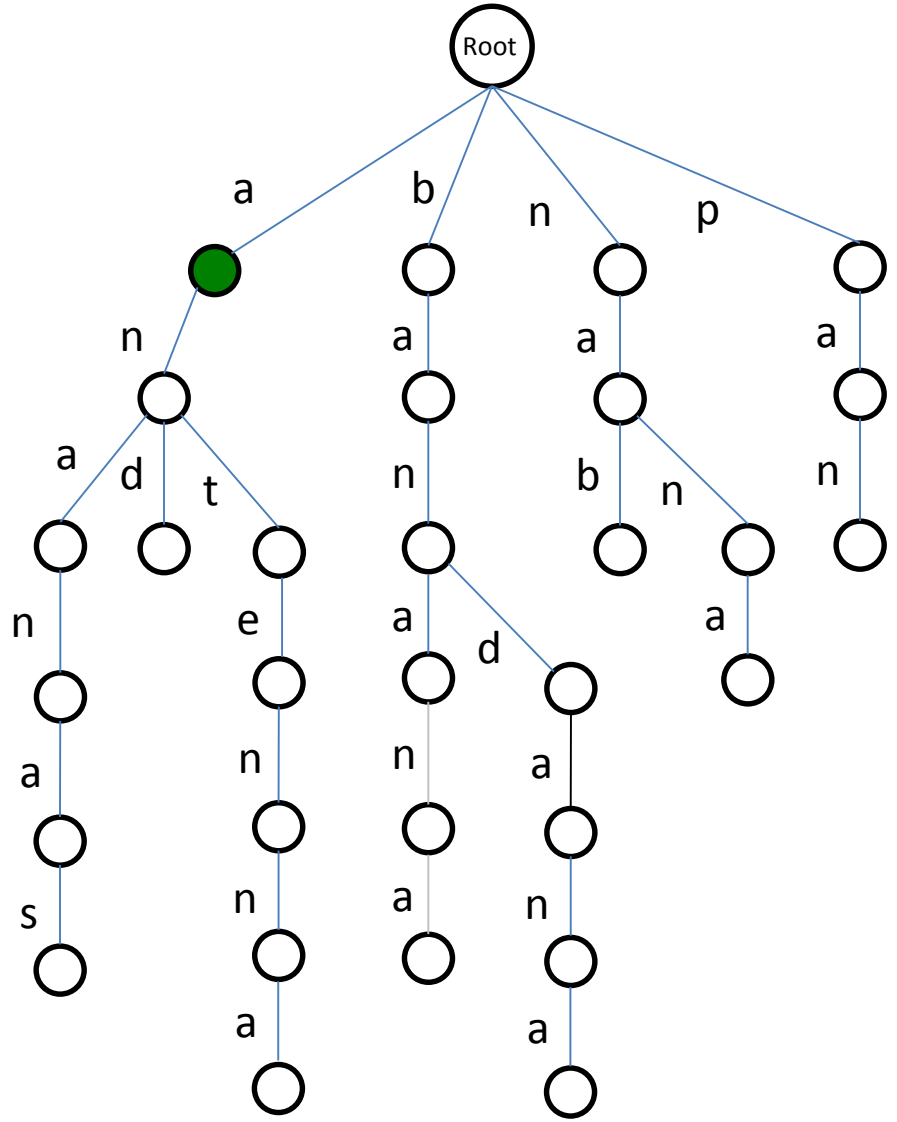
p a n a m a b a n a **n a** s



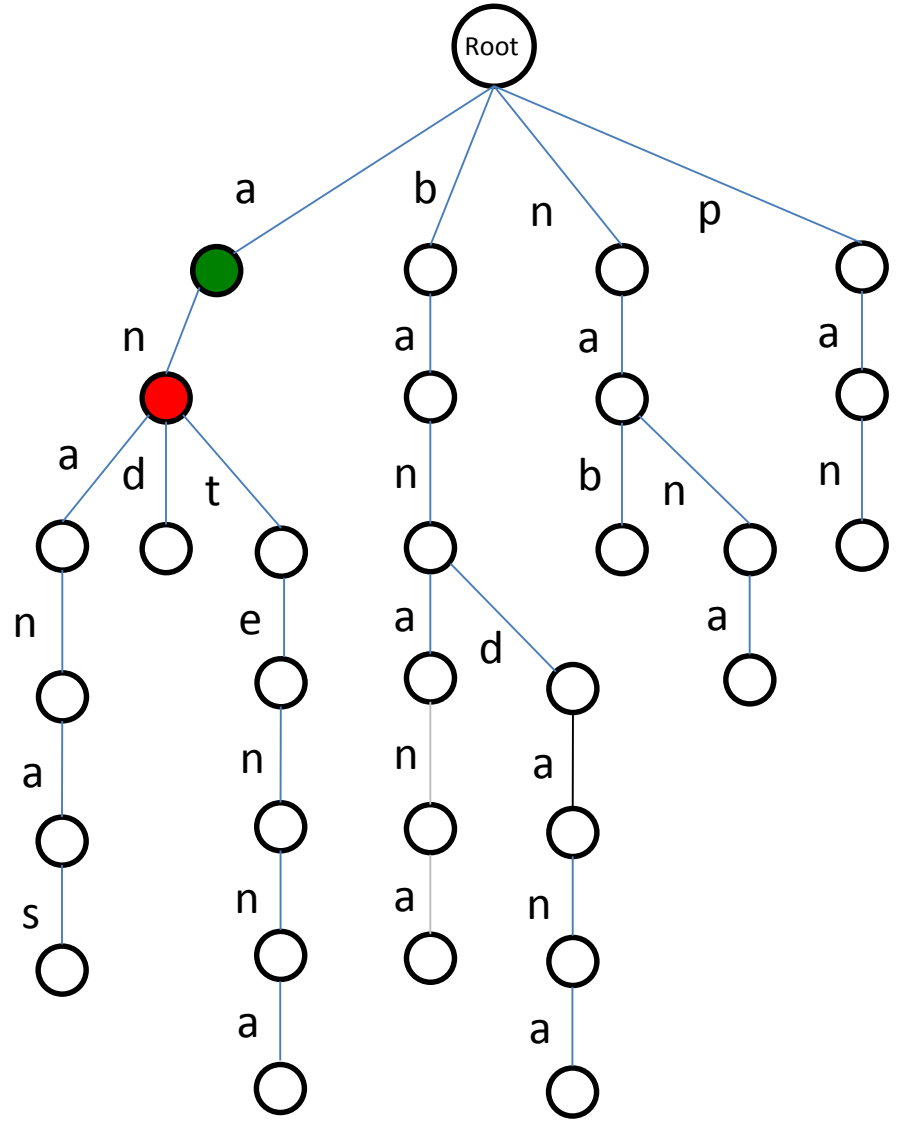
p a n a m a b a n a **n a s**



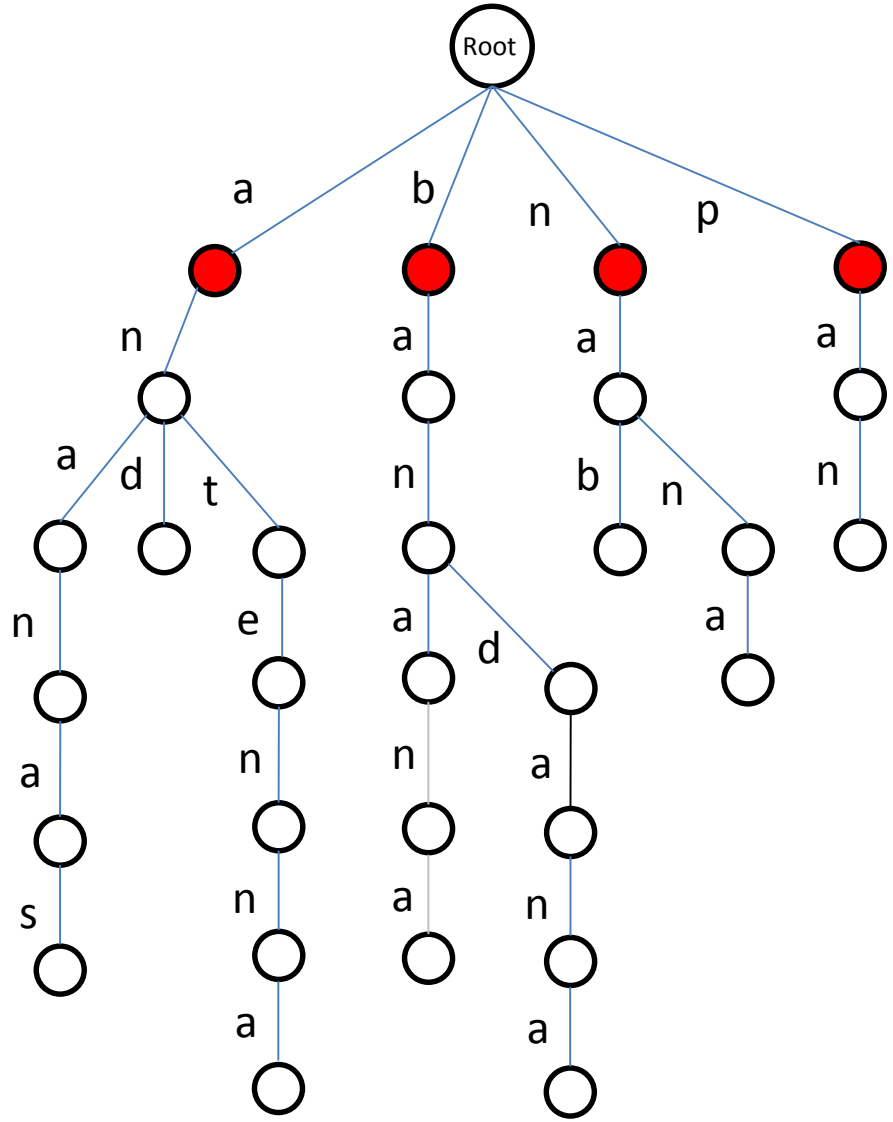
p a n a m a b a n a n **a** s



p a n a m a b a n a n **a s**



p a n a m a b a n a n a **s**



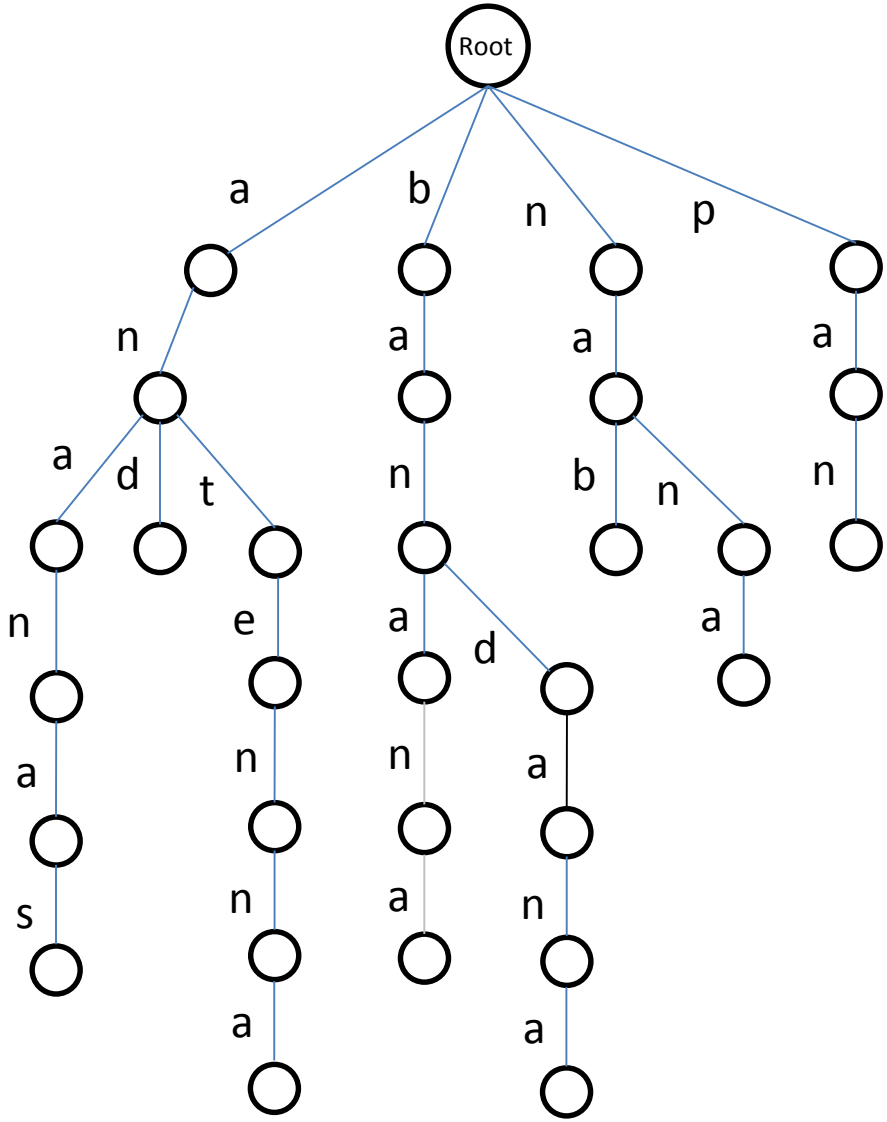
Our Bus Is Fast!

- Runtime of brute force approach:
  - O(|*Text*| • |*Patterns*|)
- Runtime of **TrieMatching**:
  - O(|*Text*| * |*LongestPattern*|)

Trie construction takes O(|*Patterns*|) time

Memory Footprint of **TrieMatching**

- Our trie has 30 edges
- # edges = O(|*Patterns*|)!
- For human genome: |*Patterns*| ≈ 10^{12}



Outline

- From Genome Sequencing to Pattern Matching
- Brute Force Approach to Pattern Matching
- Herding Patterns into Trie
- **Herding Text into Suffix Trie**
- From Suffix Tries to Suffix Trees

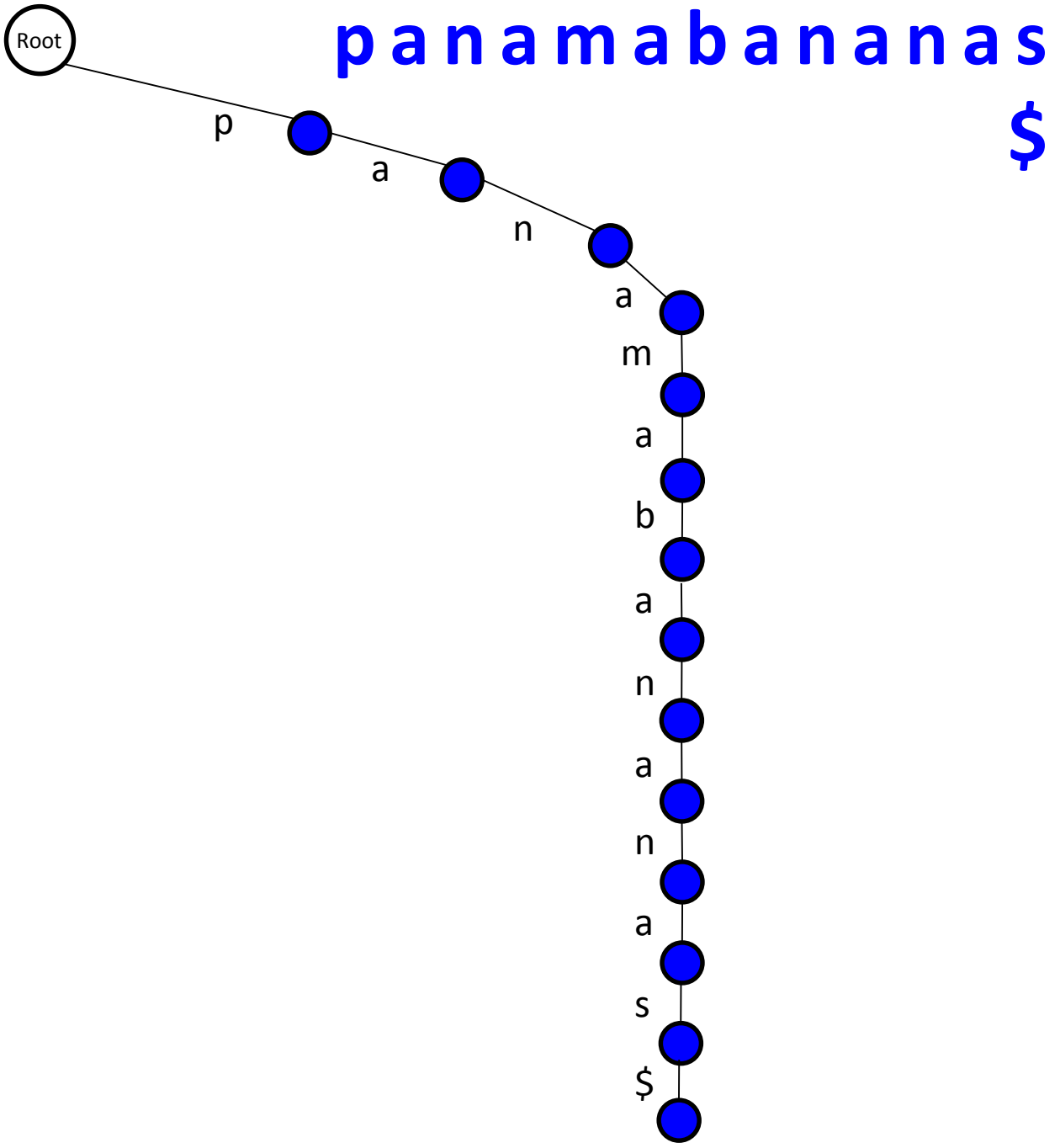
New Idea: Packing *Text* onto a Bus

- Generate all suffixes of *Text*
- Form a trie out of these suffixes (**suffix trie**)
- For each *Pattern*, check if it can be spelled out from the root downward in the suffix trie

p a n a m a b a n a n a s

p a n a m a b a n a n a s $

Adding “$” sign in the end (we’ll explain later why)


Root
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p a n a m a b a n a n a s
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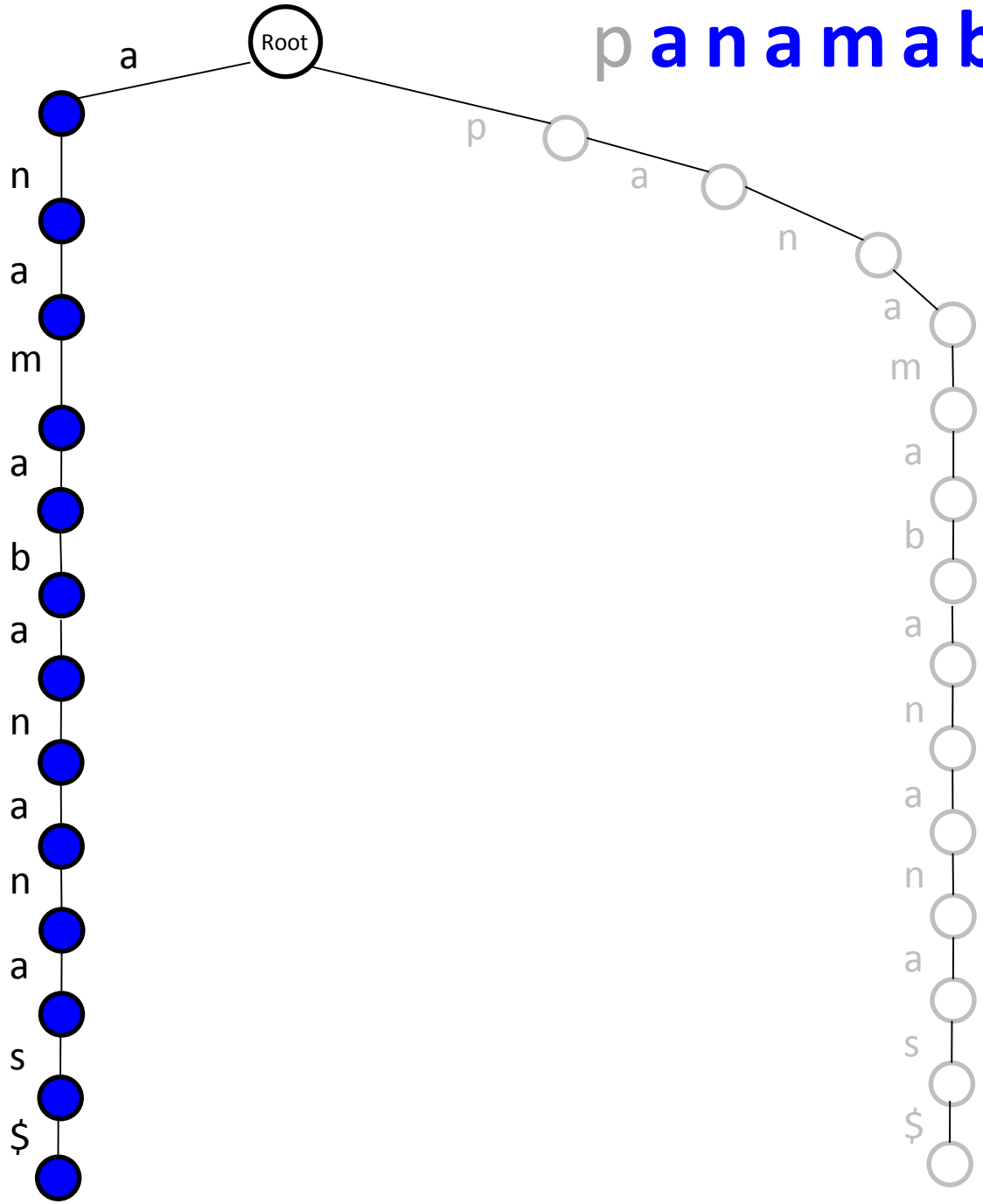
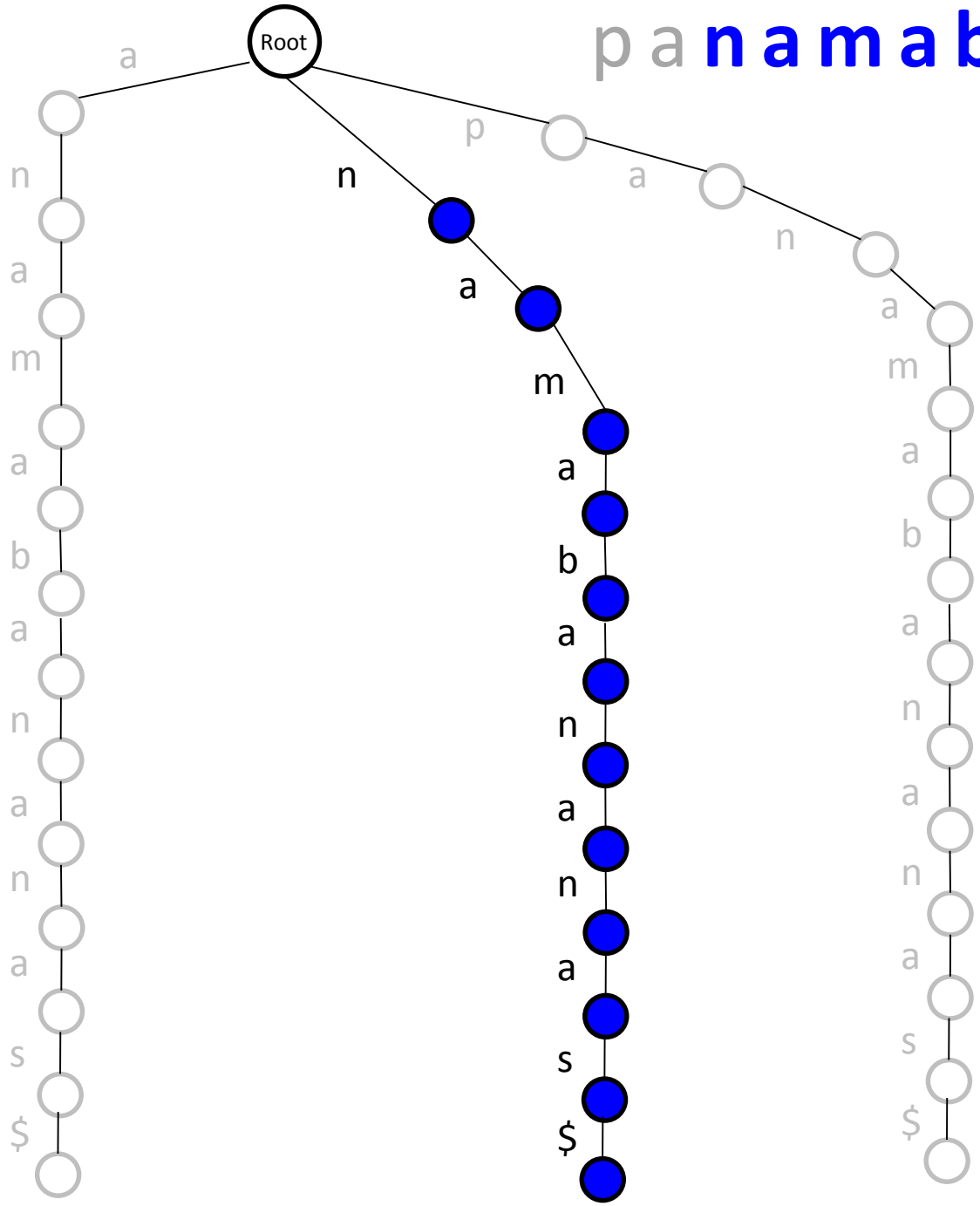


p a n a m a b a n a n a s $



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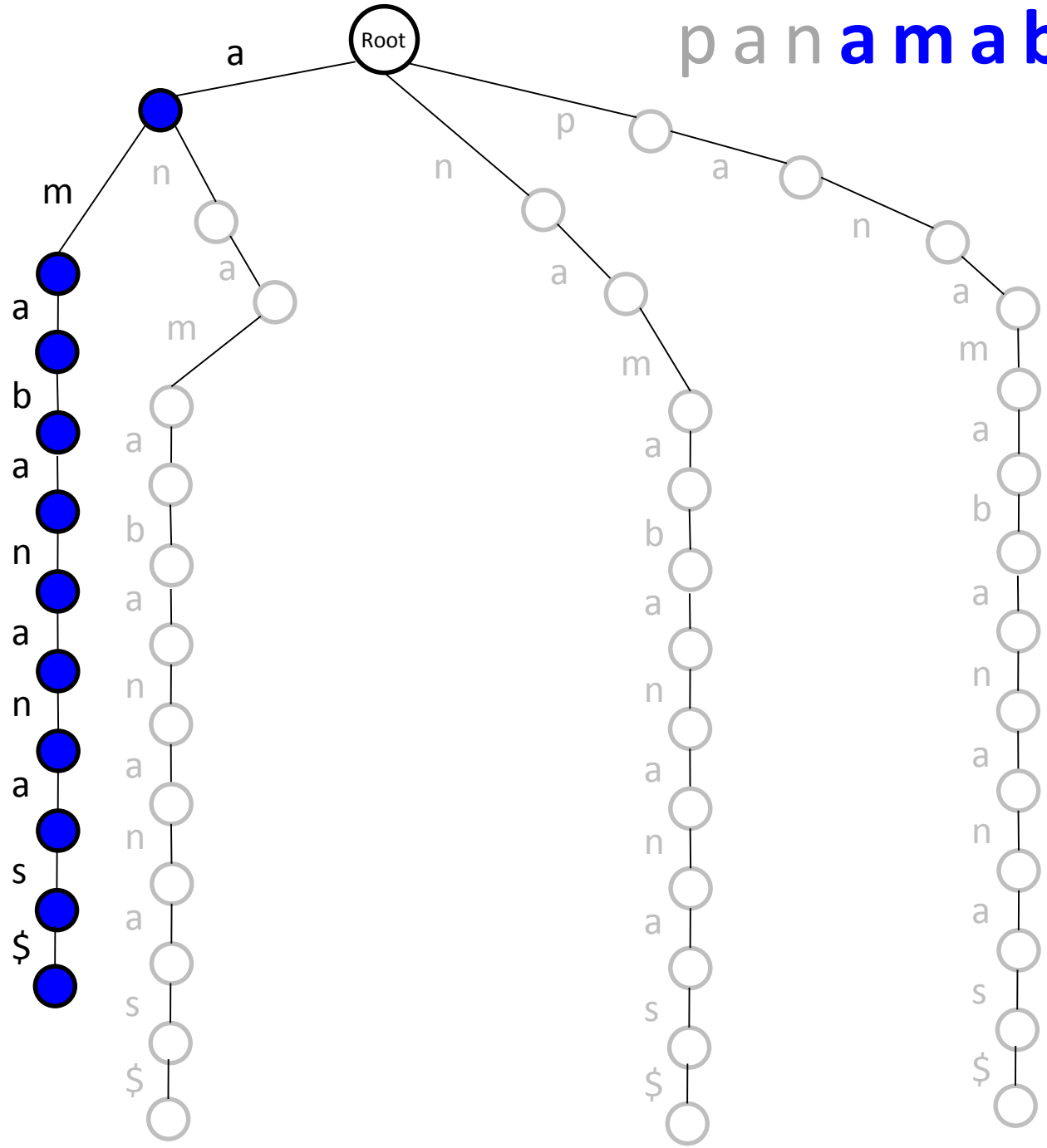

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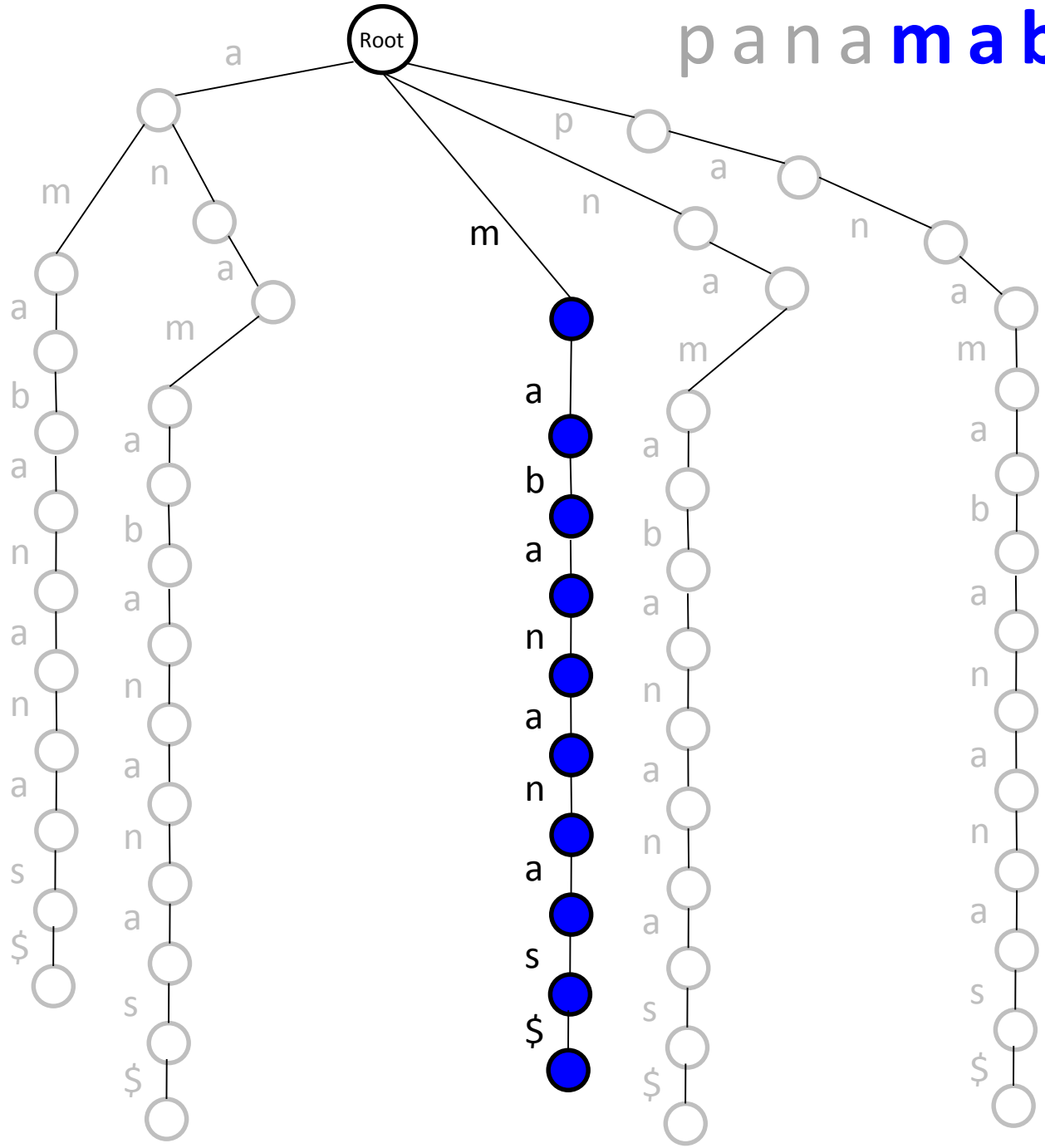
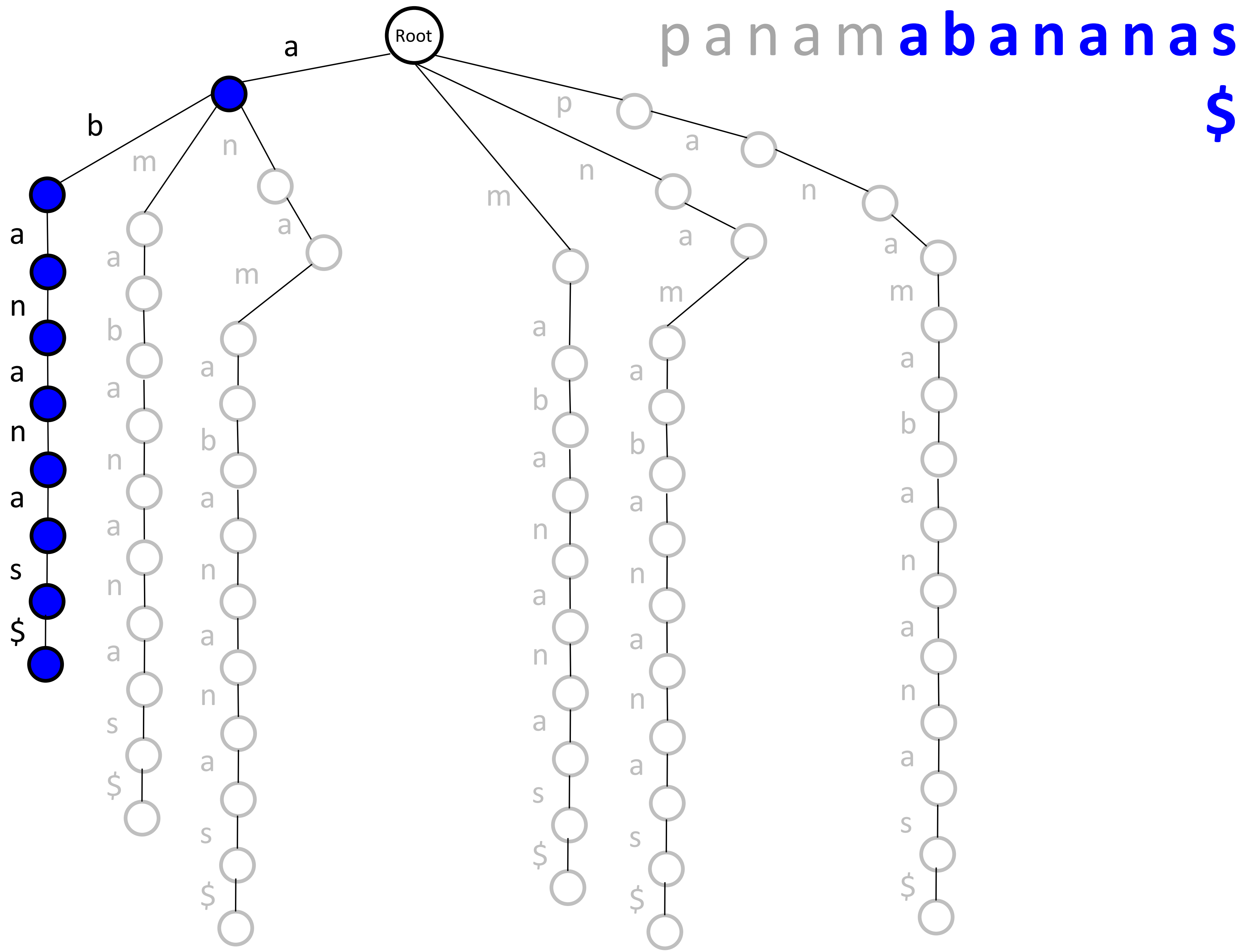
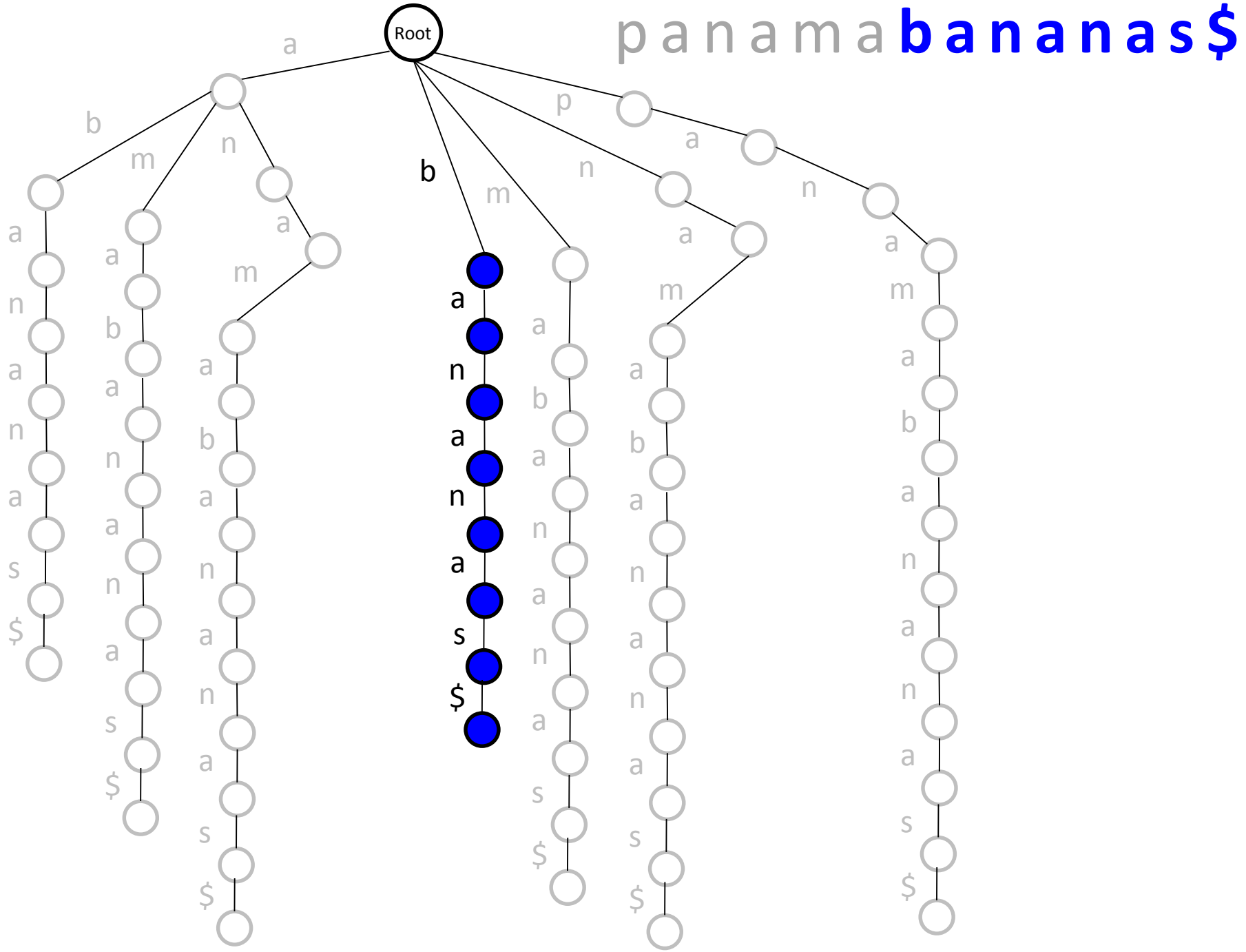
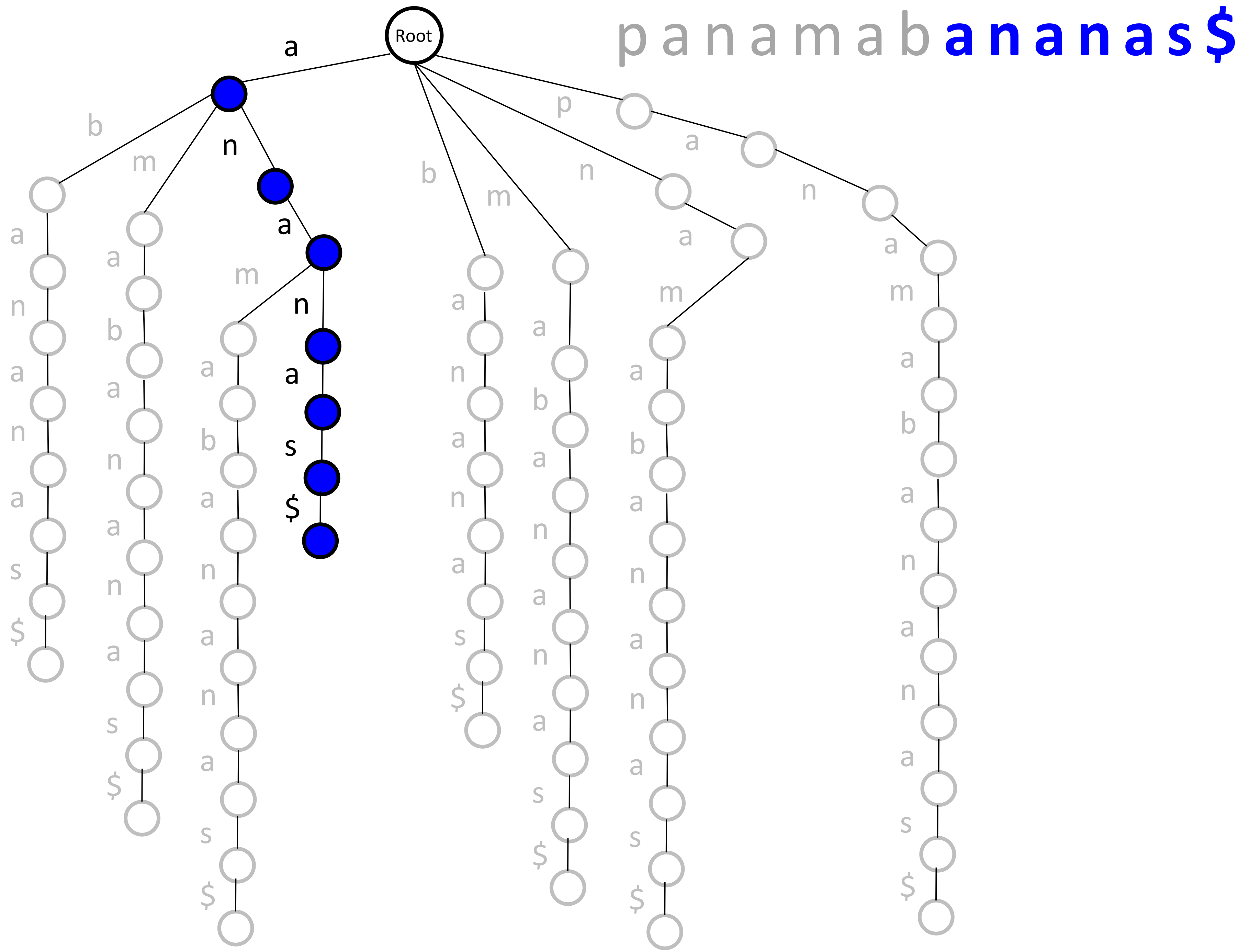


p a n a **m a b a n a n a s $**


p a n a m a b a n a n a s $
Root


Root
panamabananas$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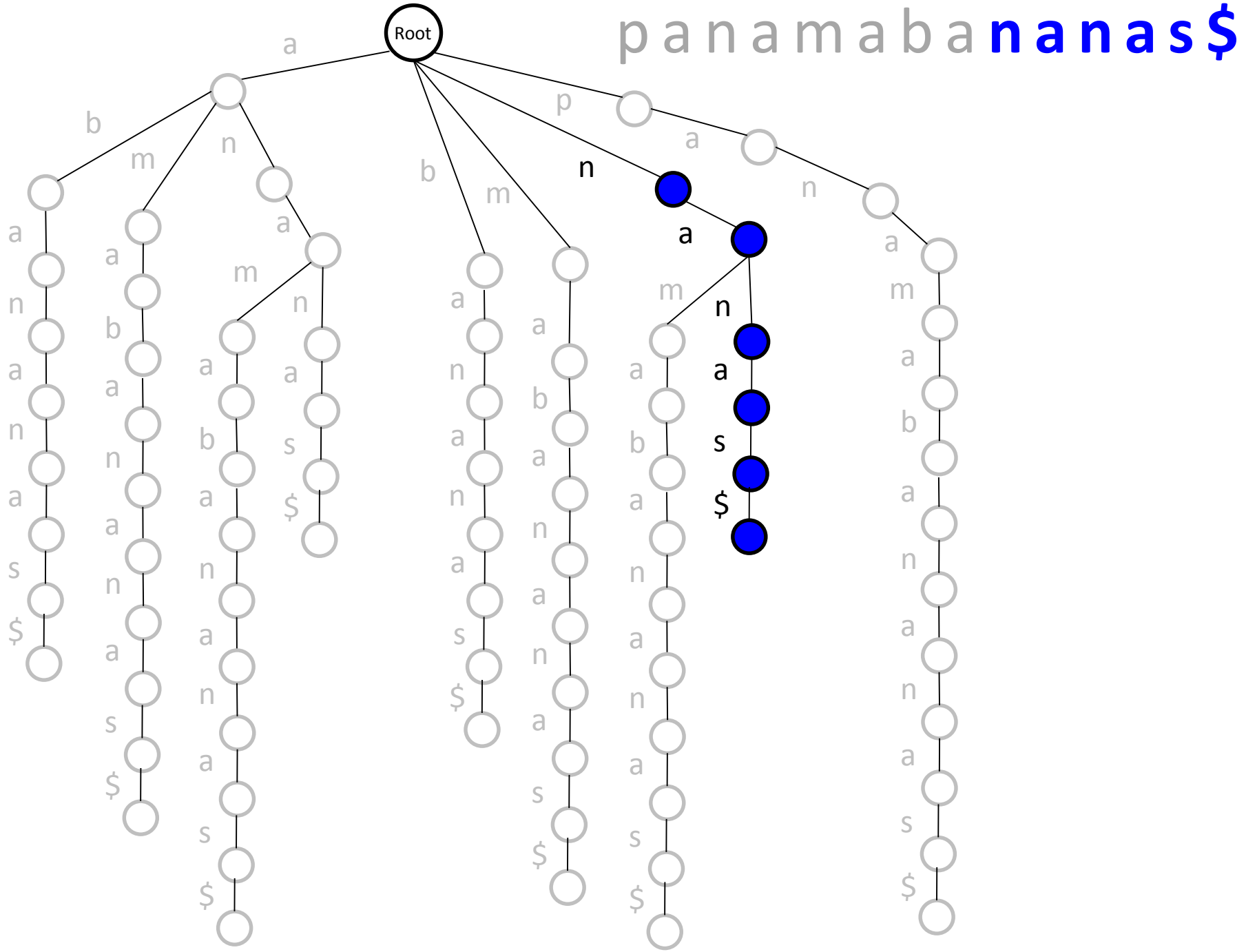
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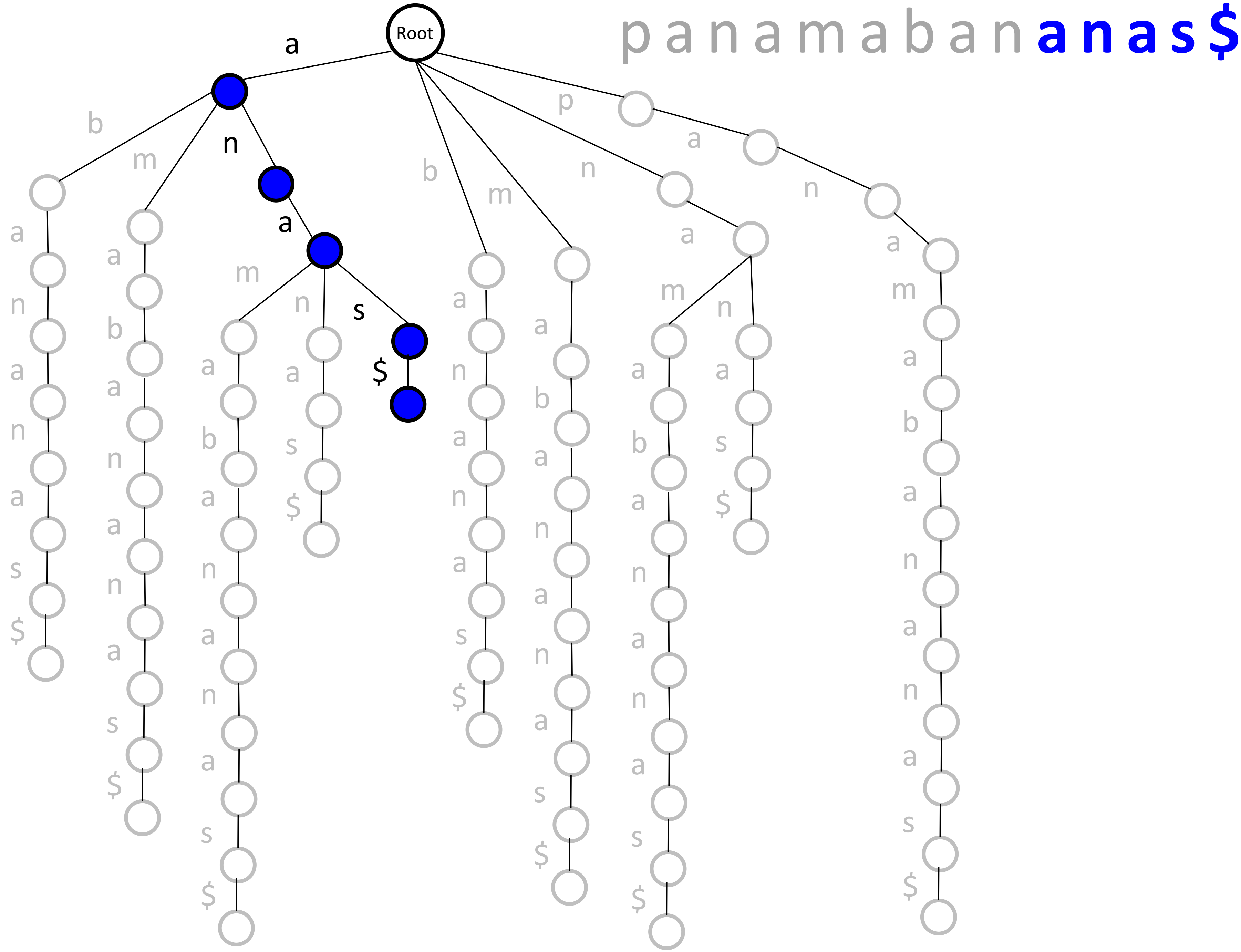
p a n a m a b a n a n a s $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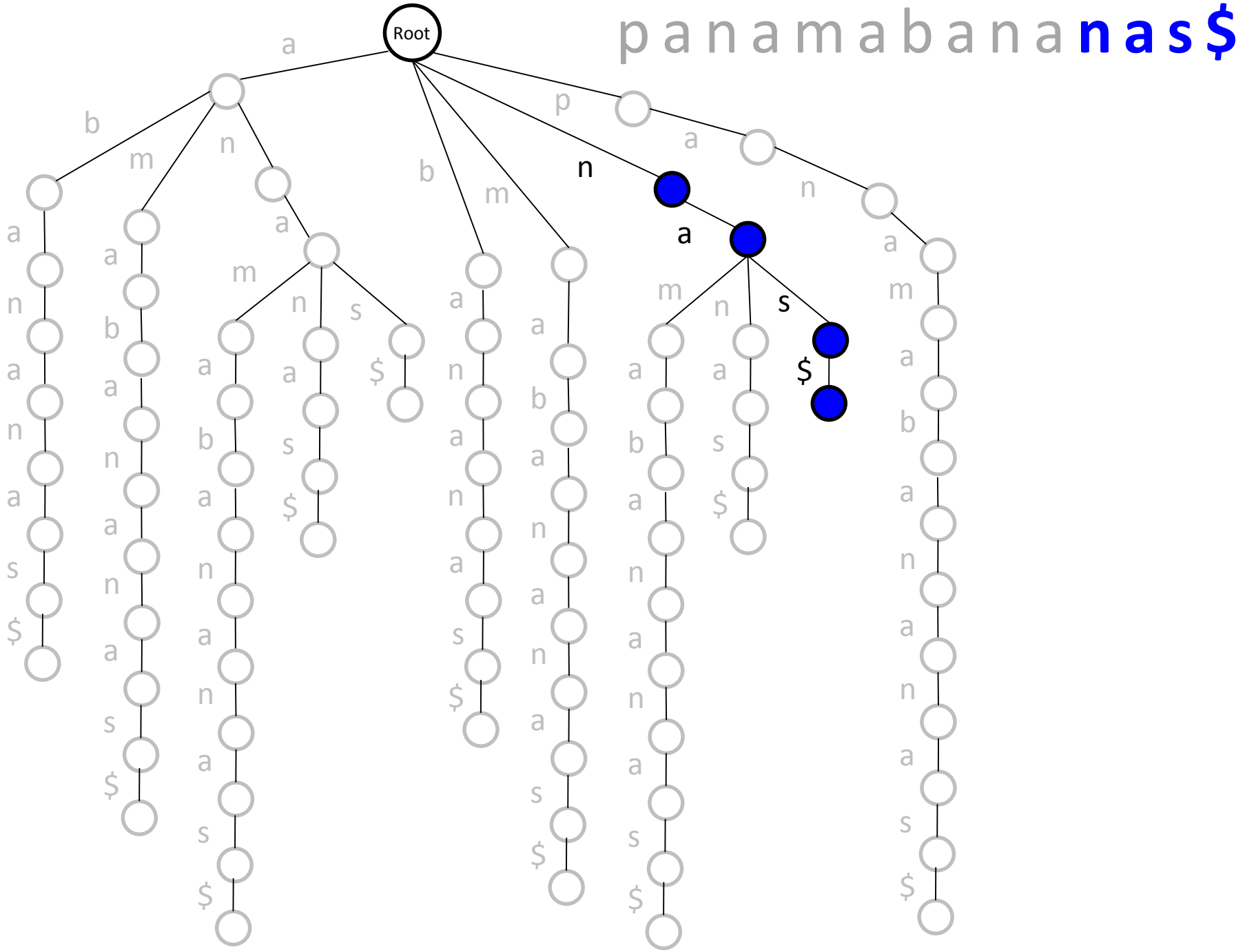
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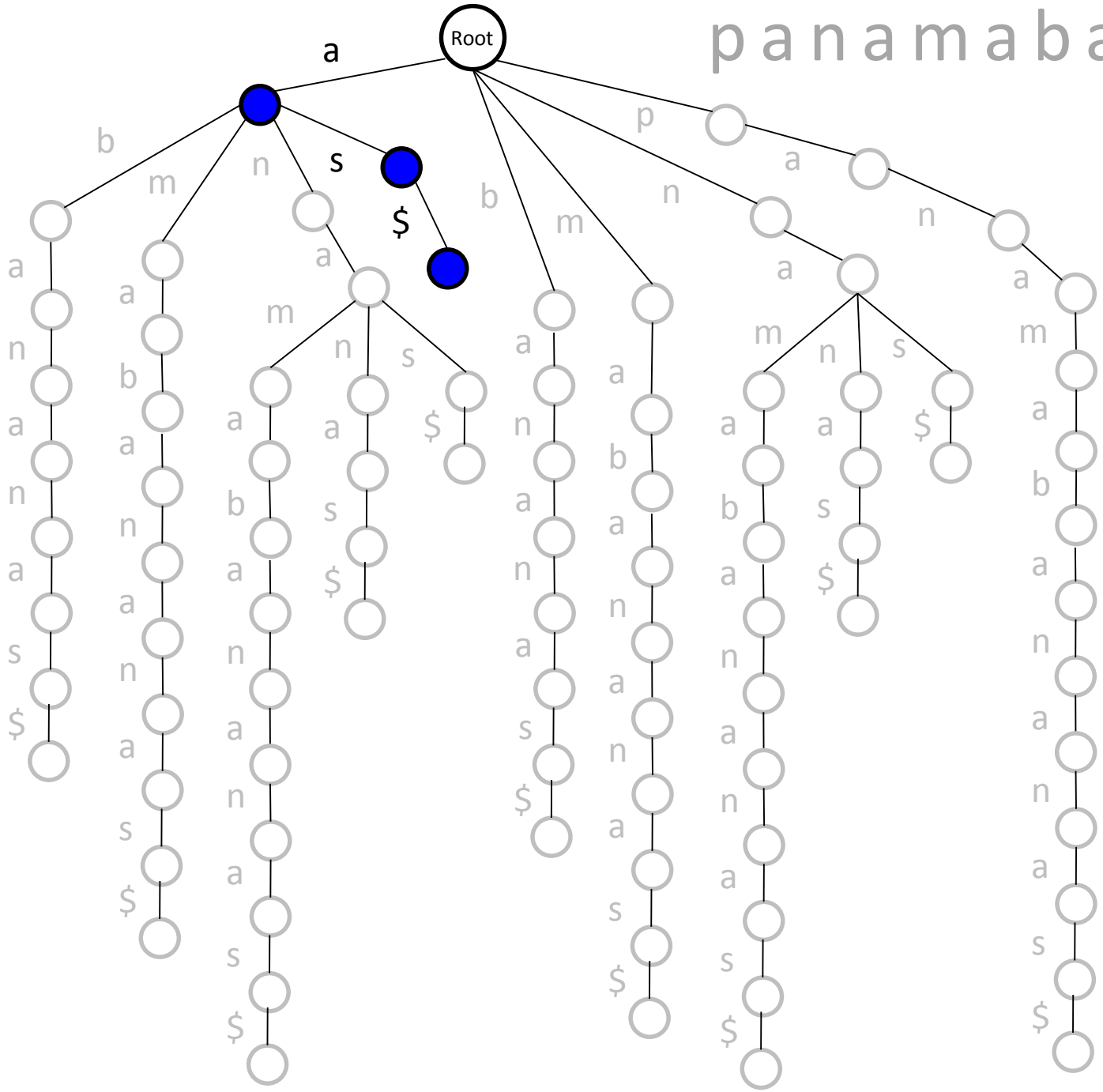
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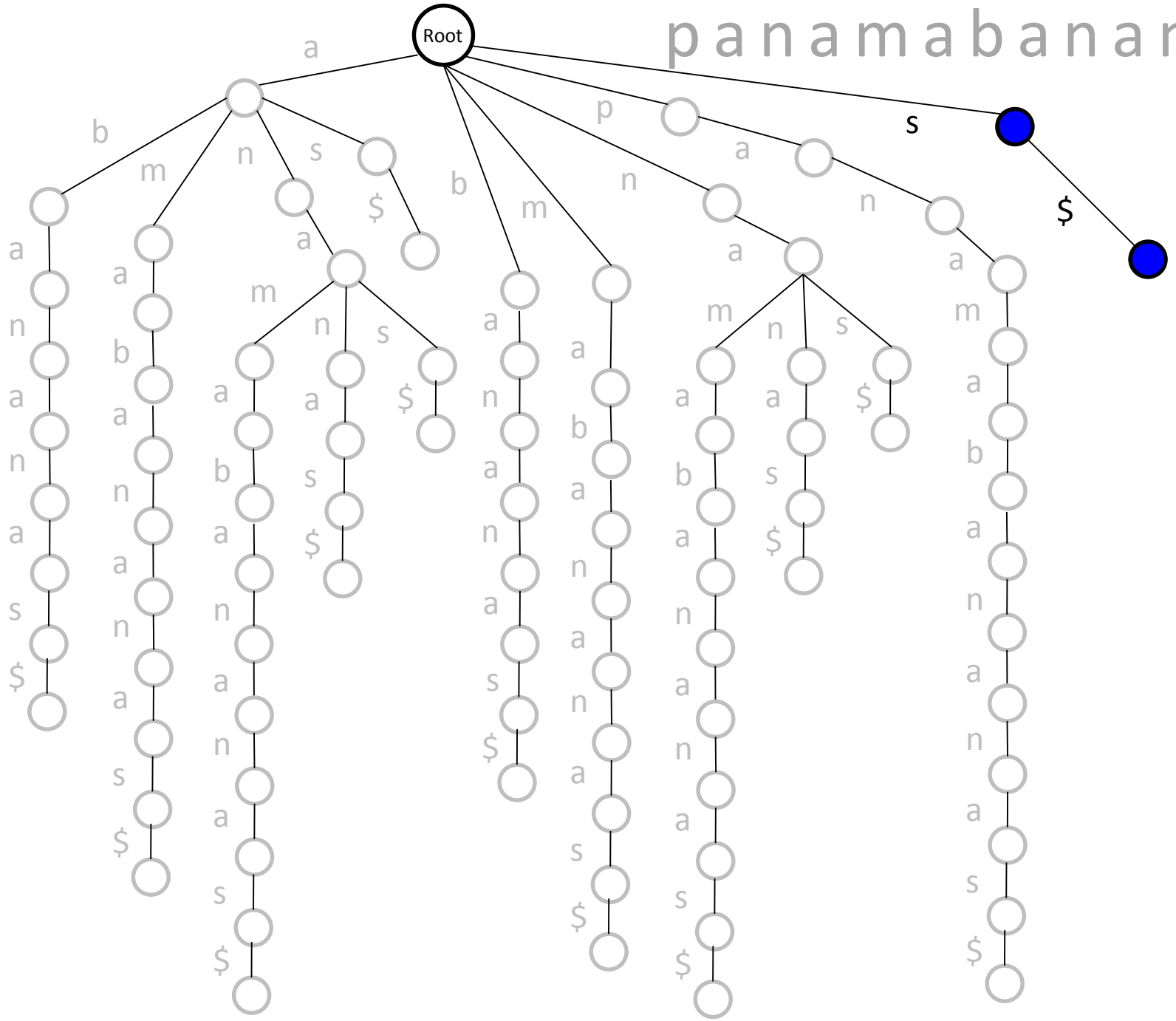
panamabanana$
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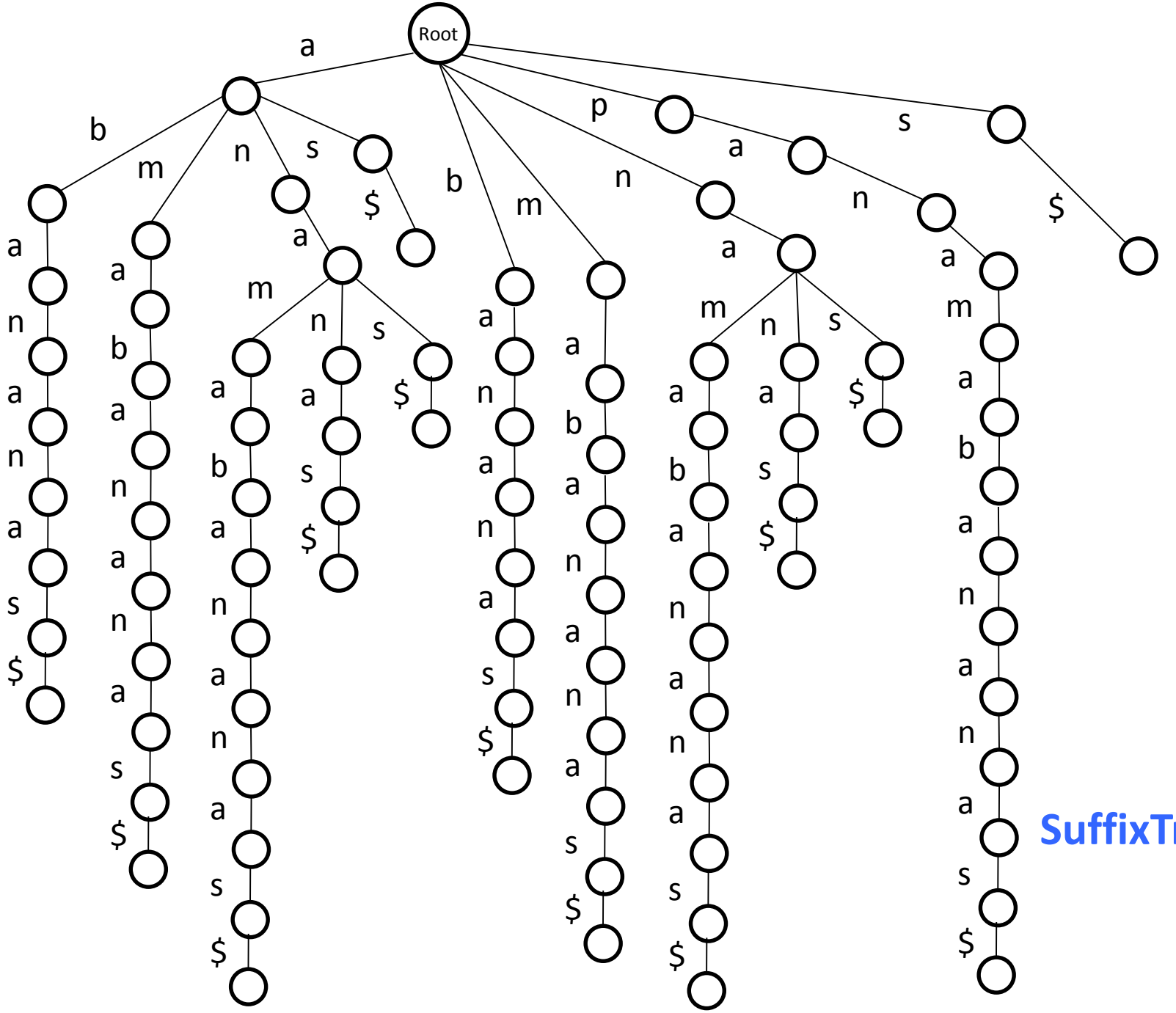
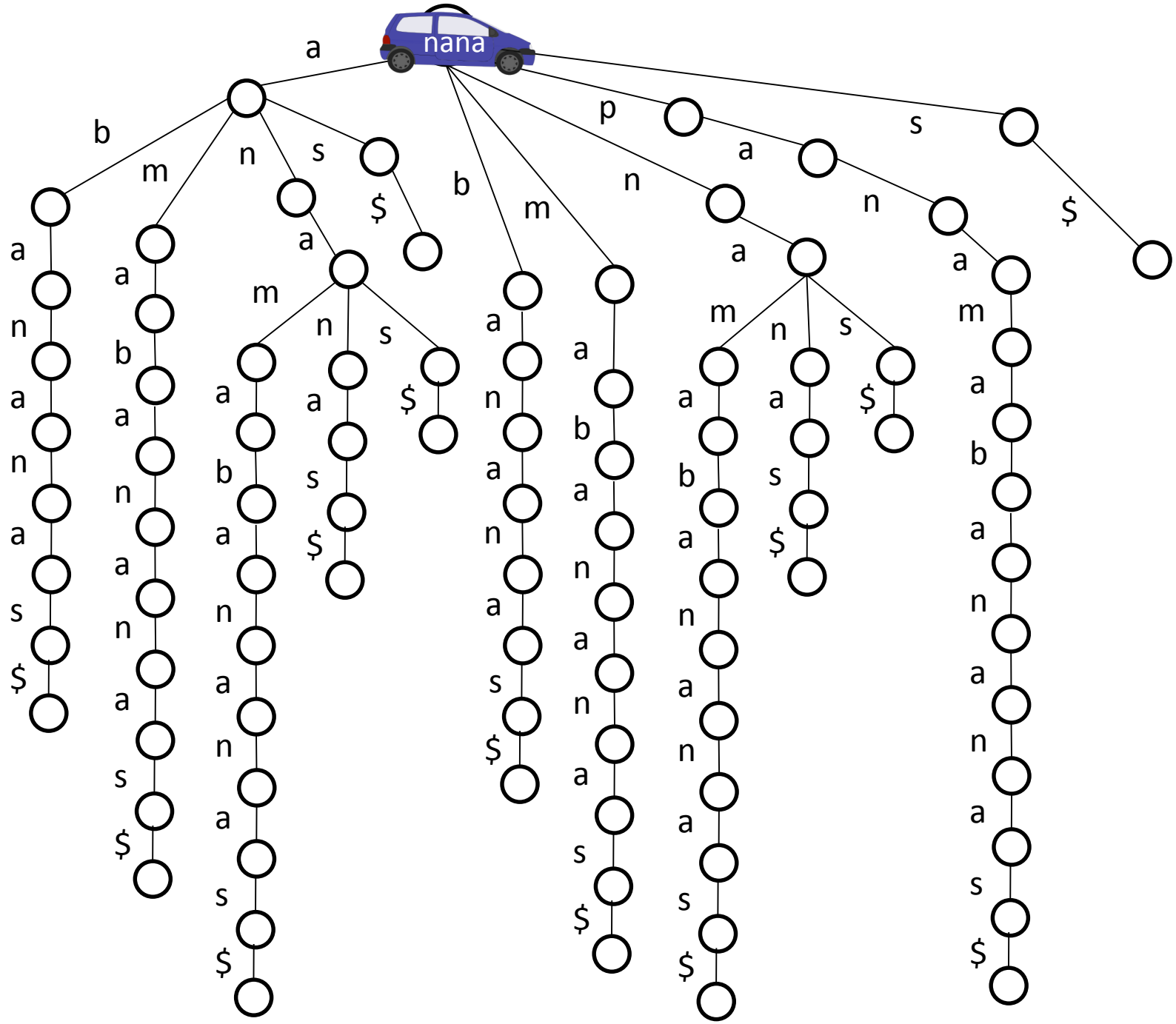
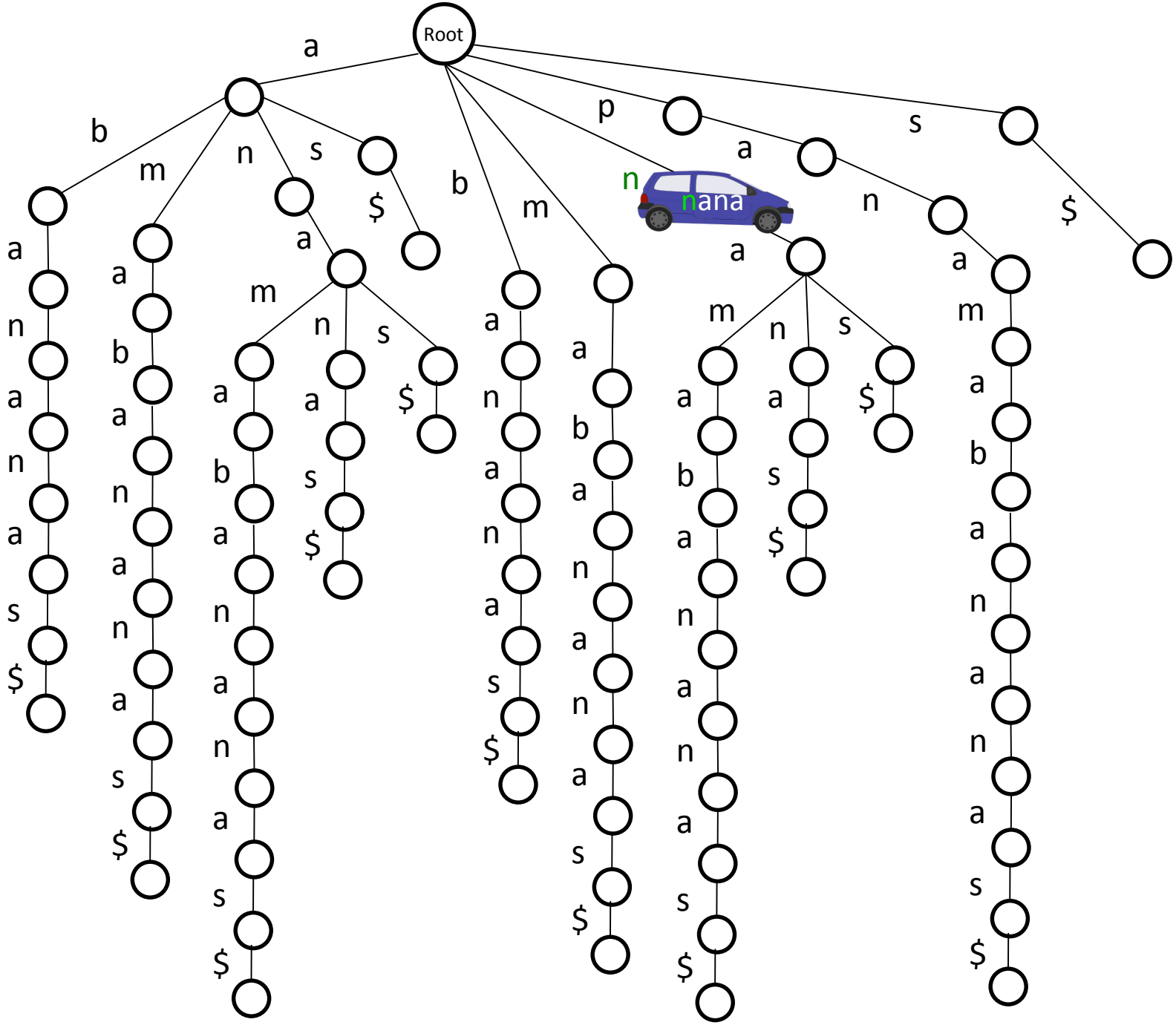

Root
SuffixTrie(*Text*)


nana


Root
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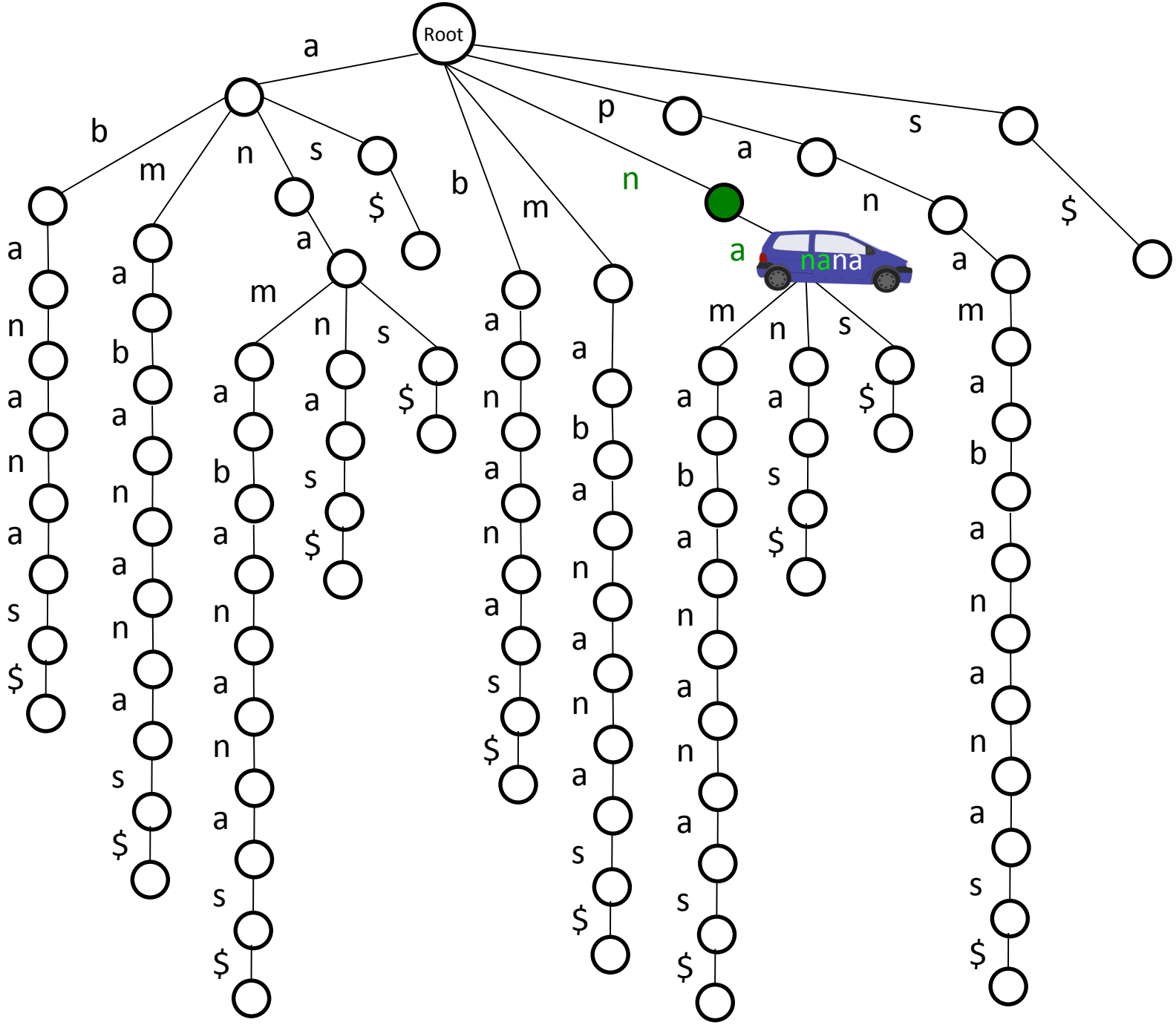
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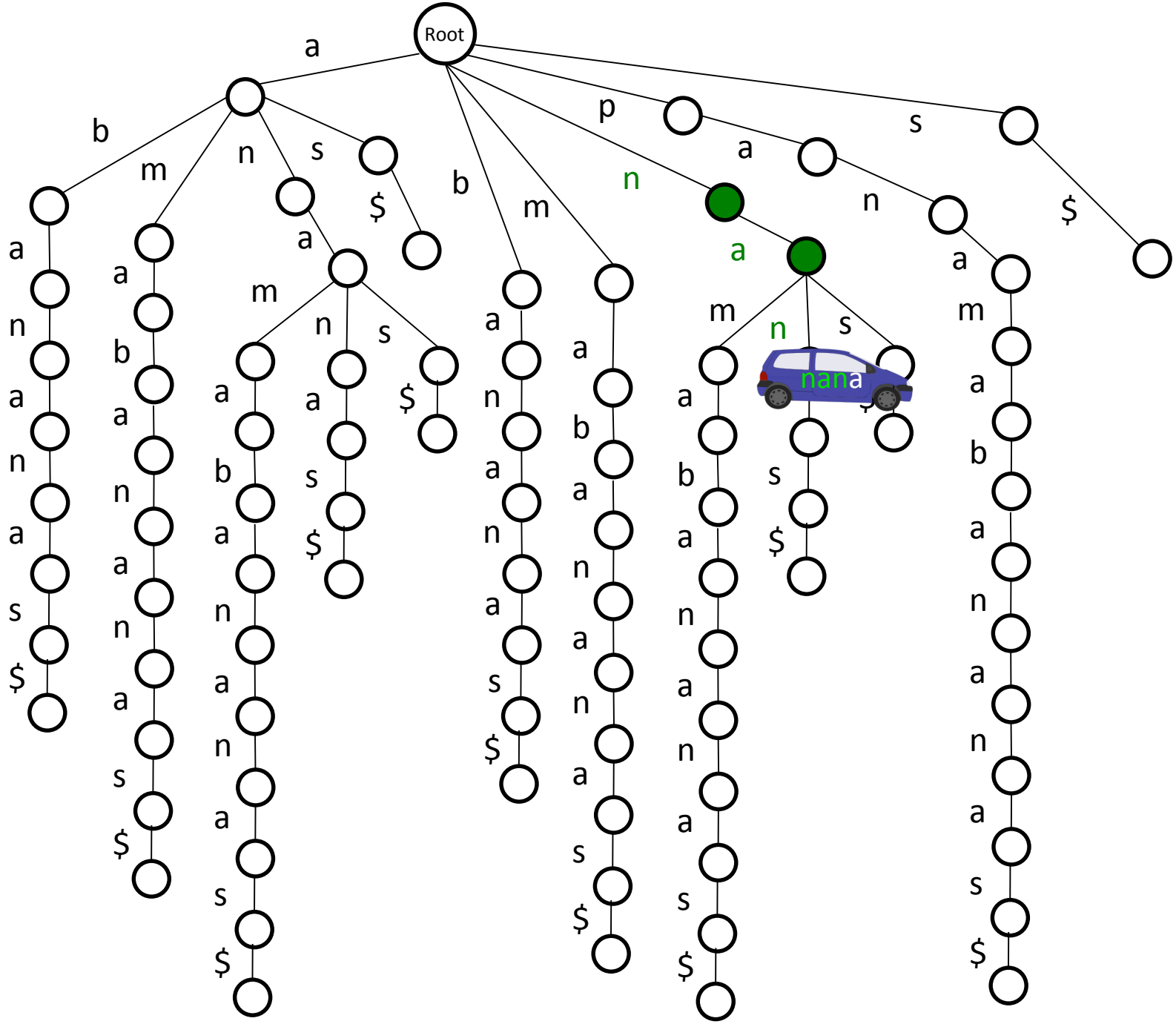
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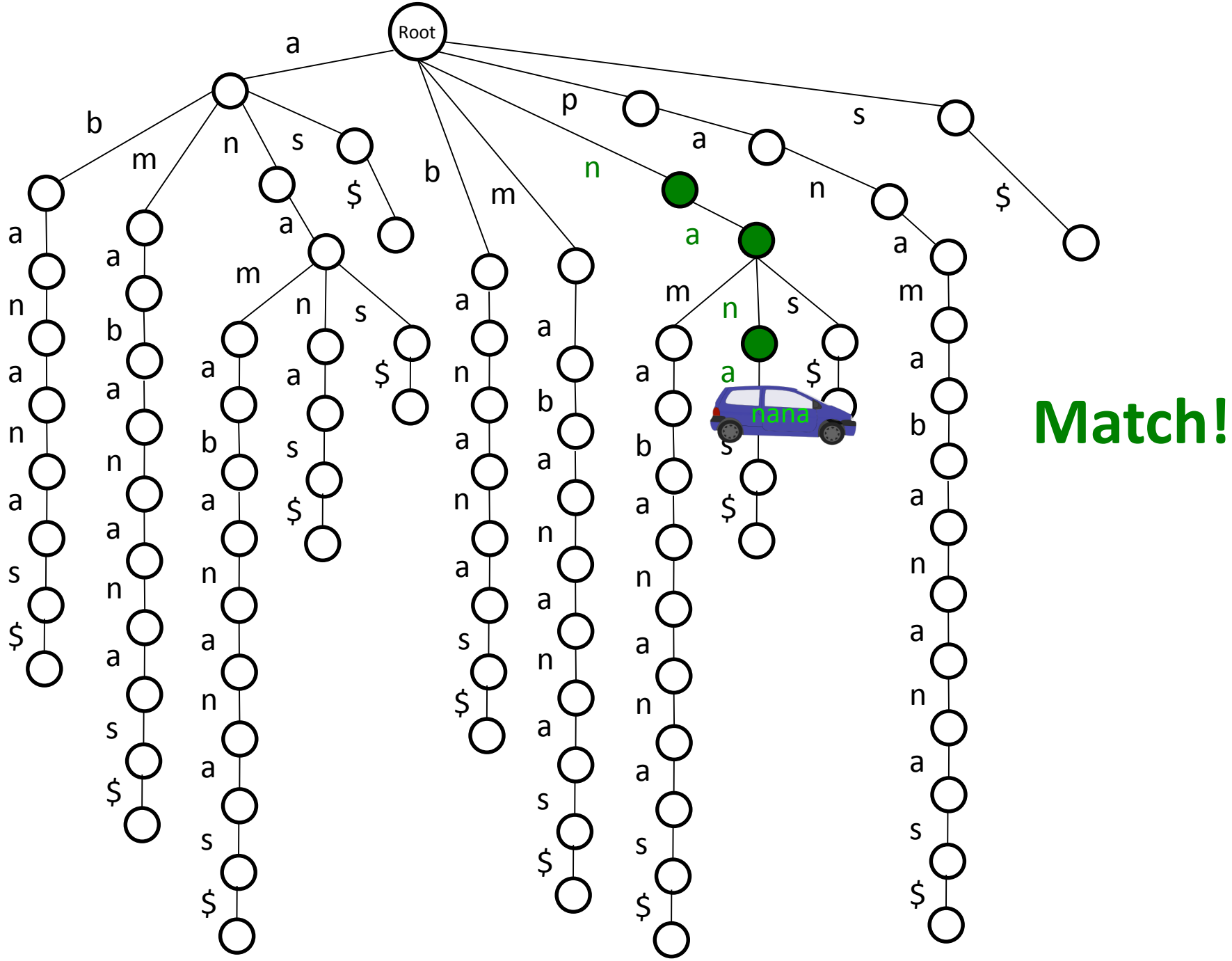
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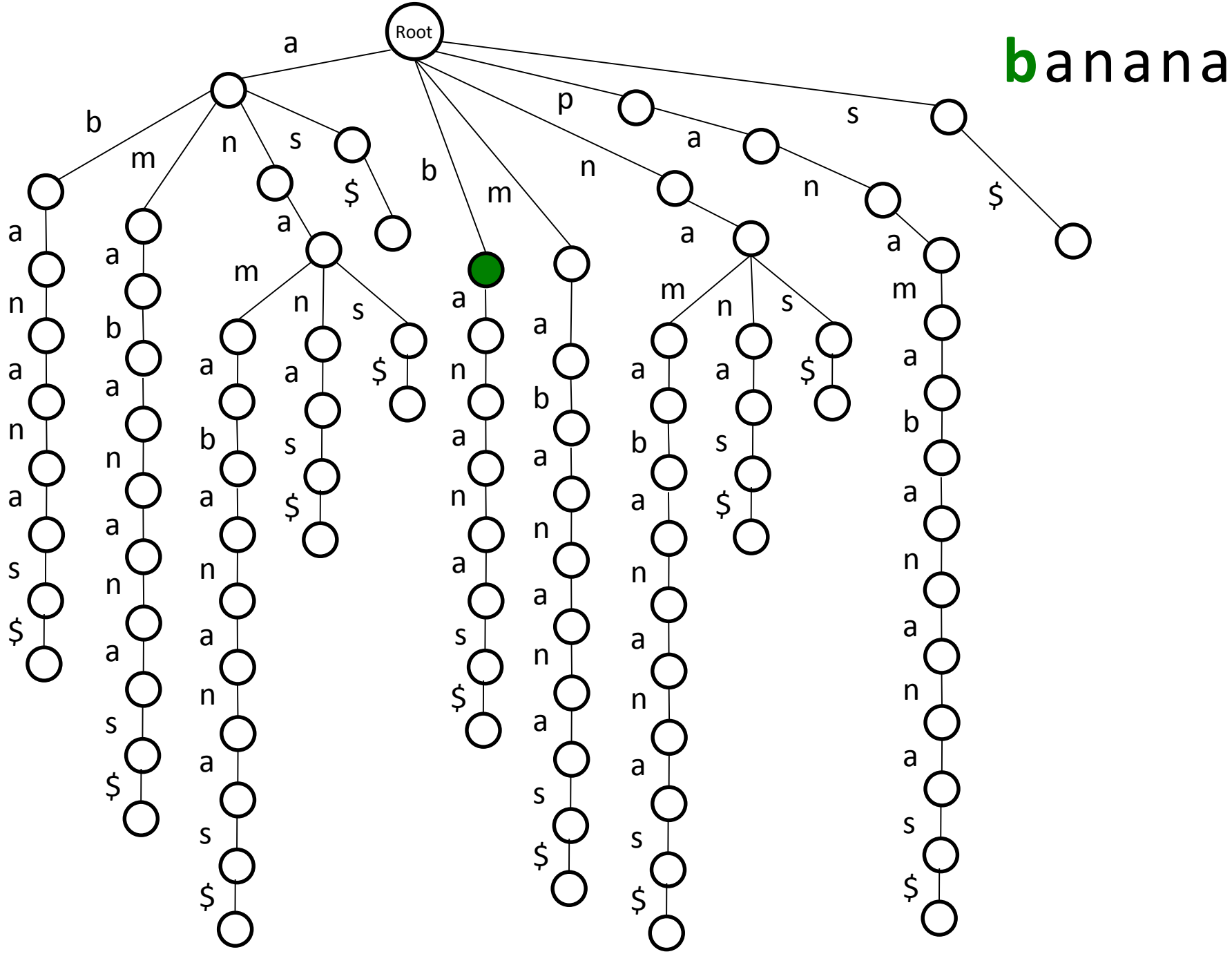
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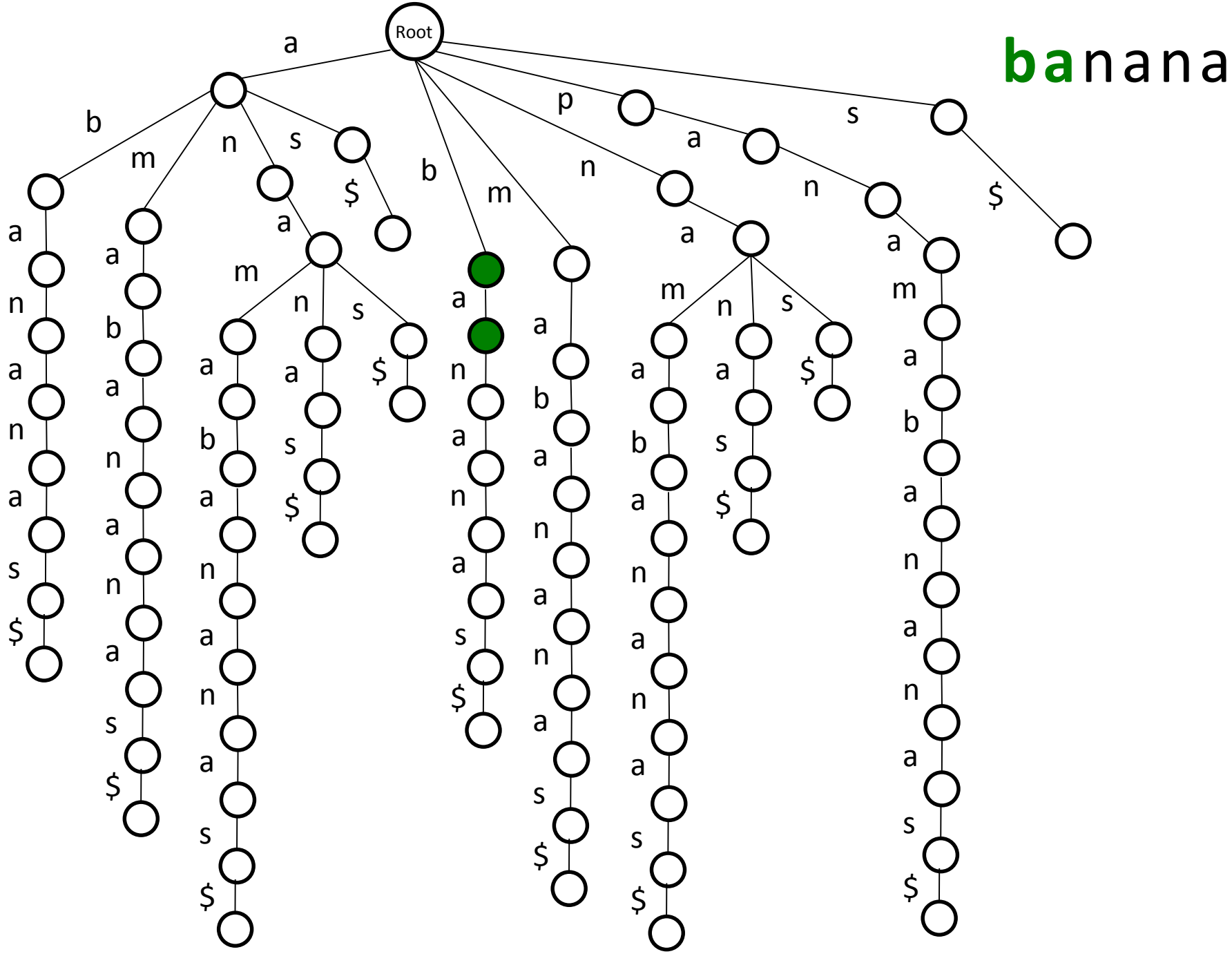
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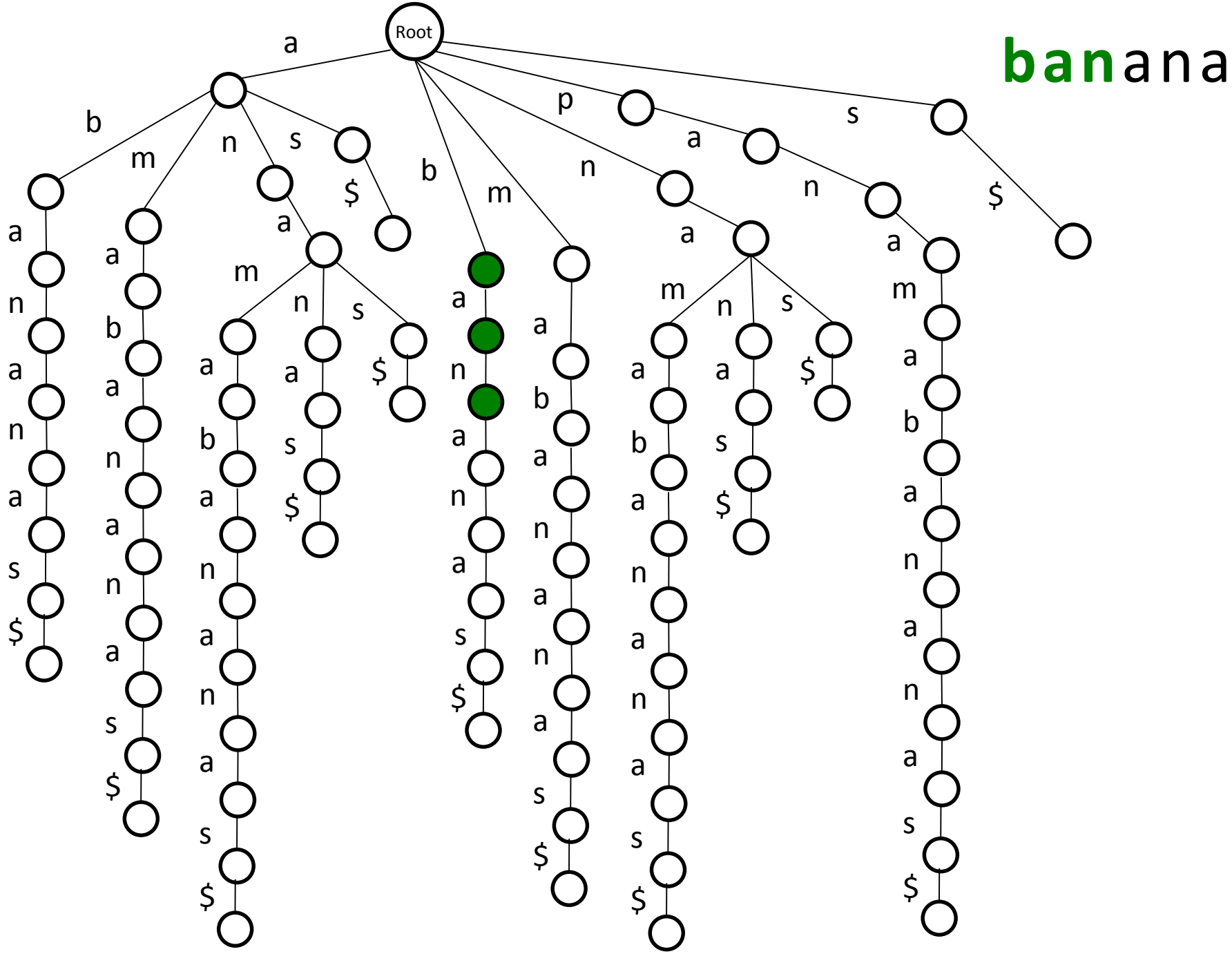
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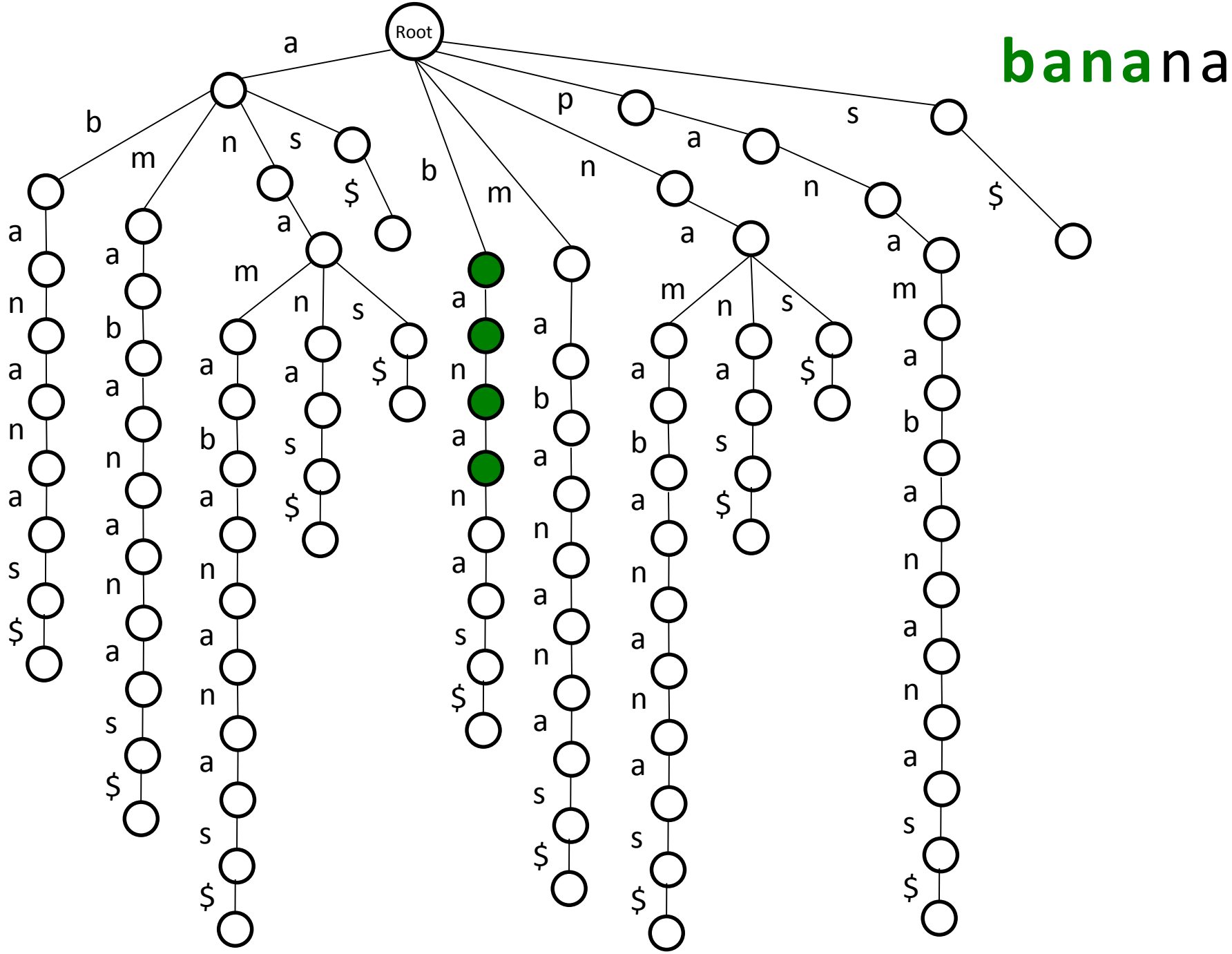
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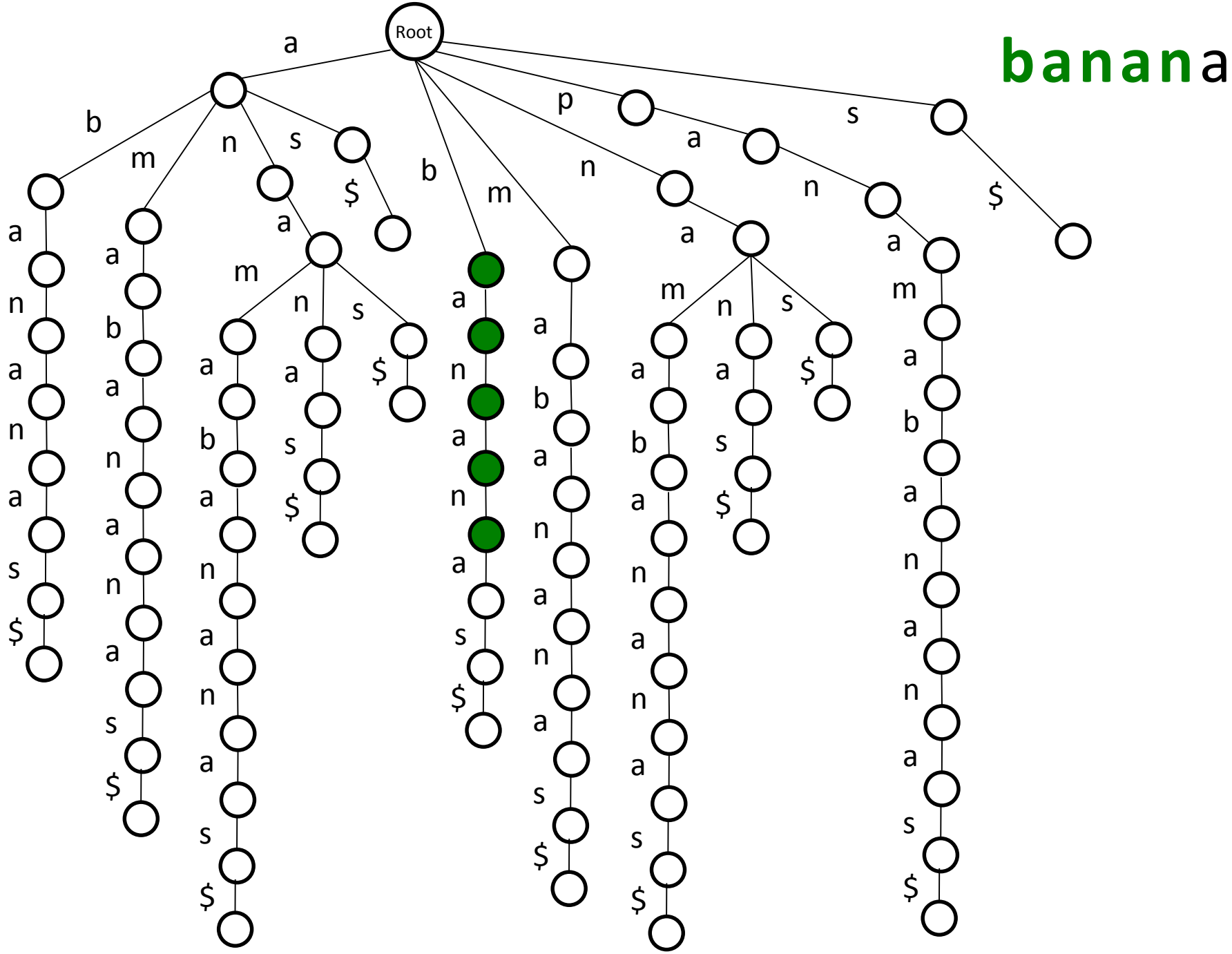
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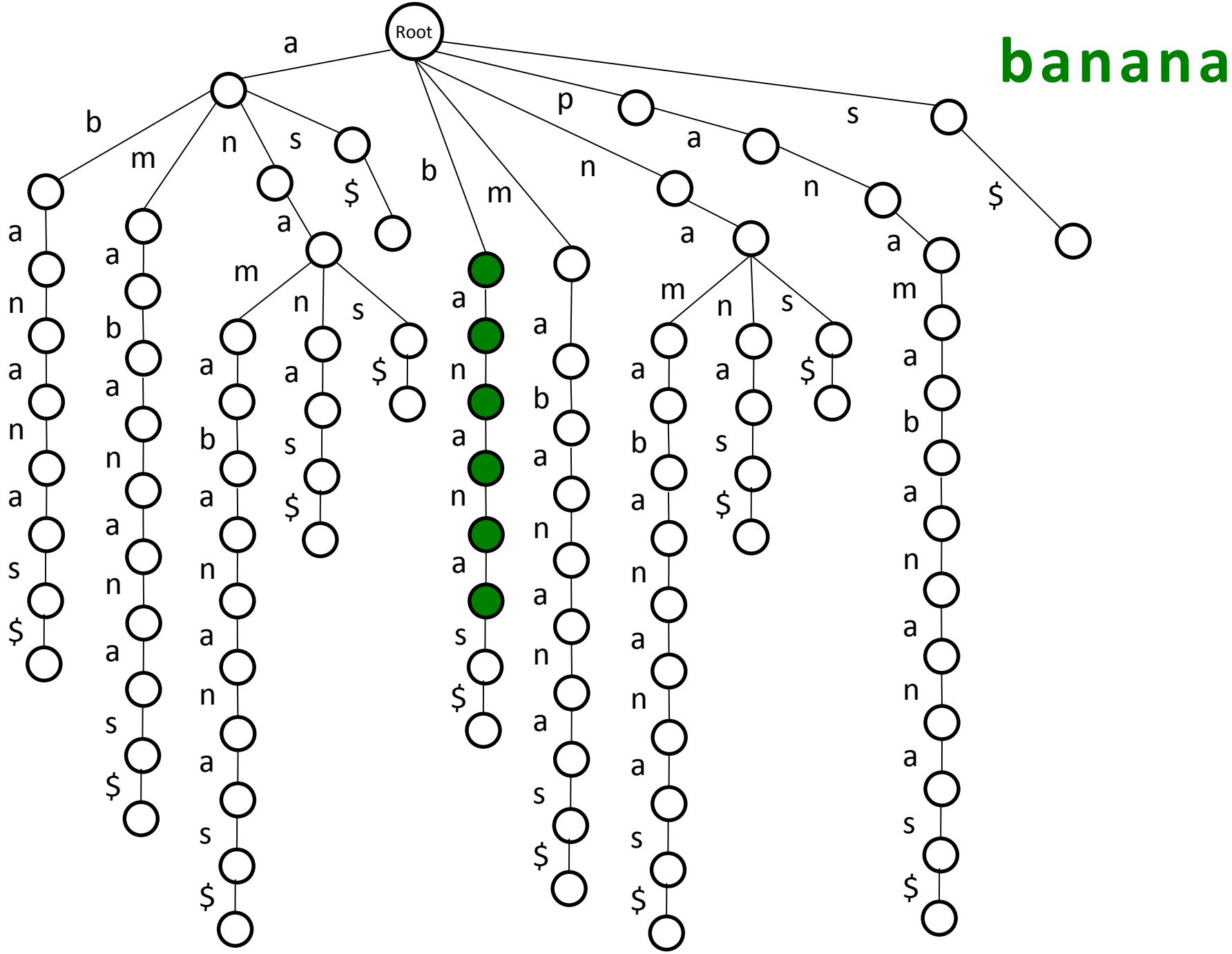
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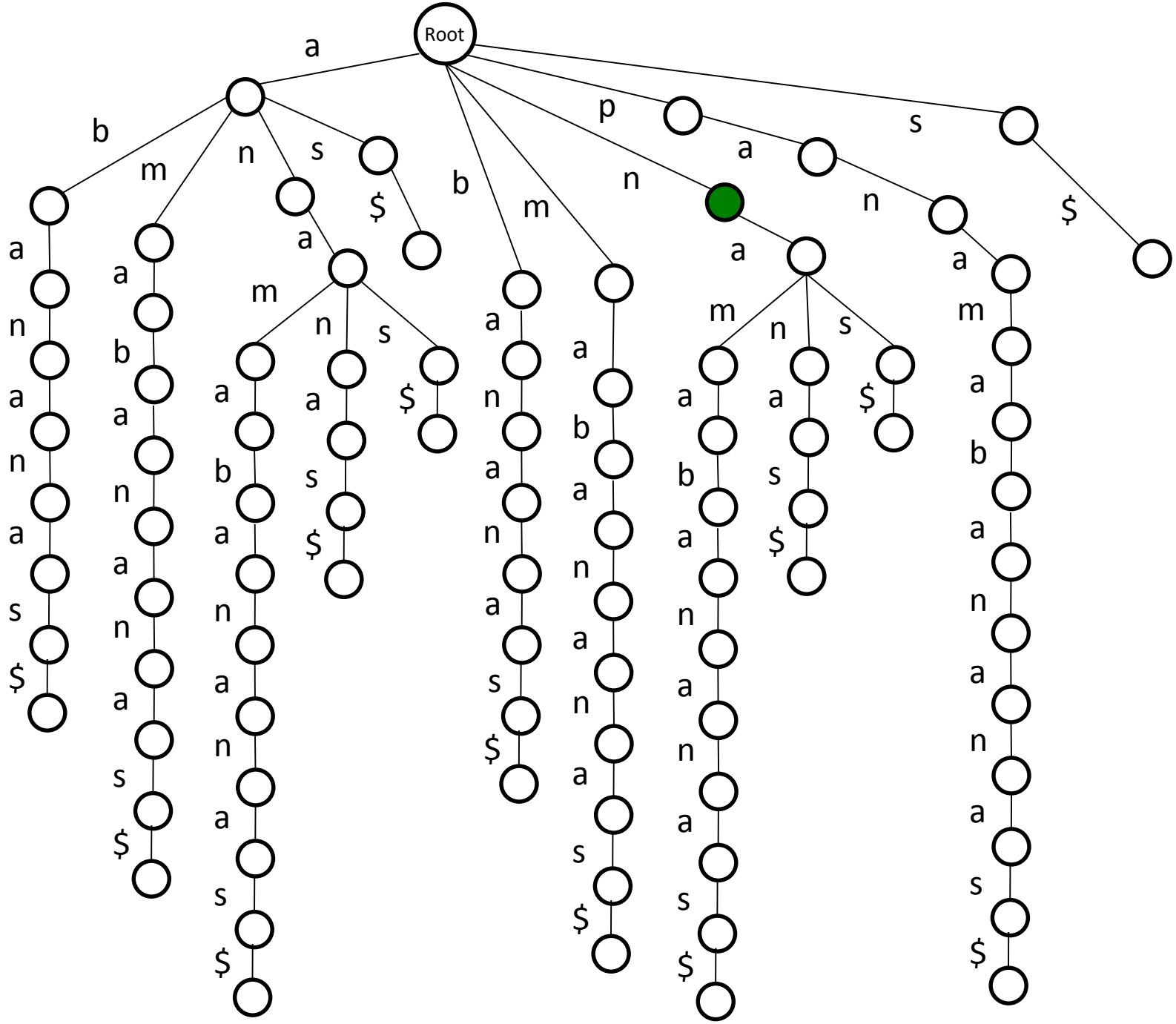
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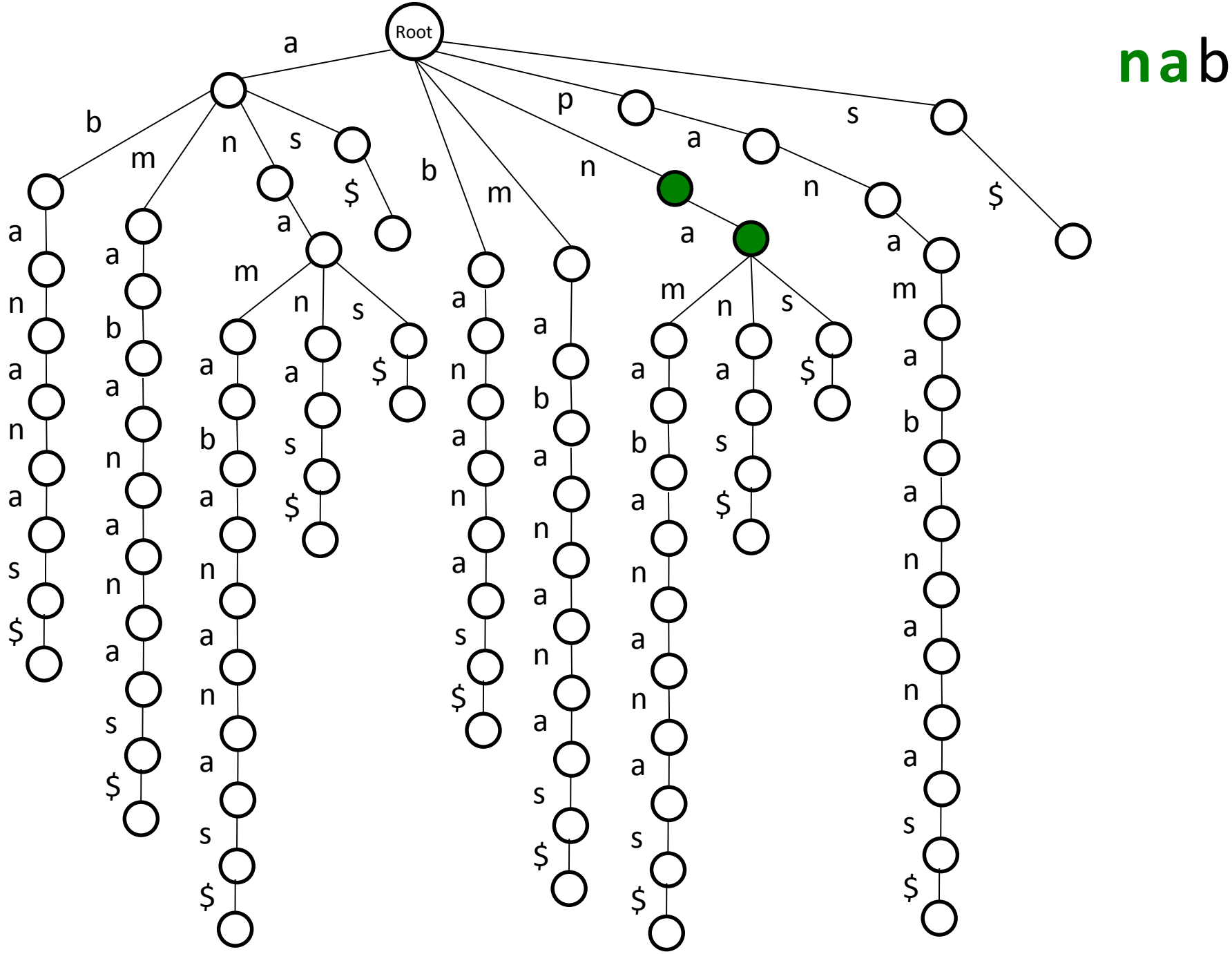
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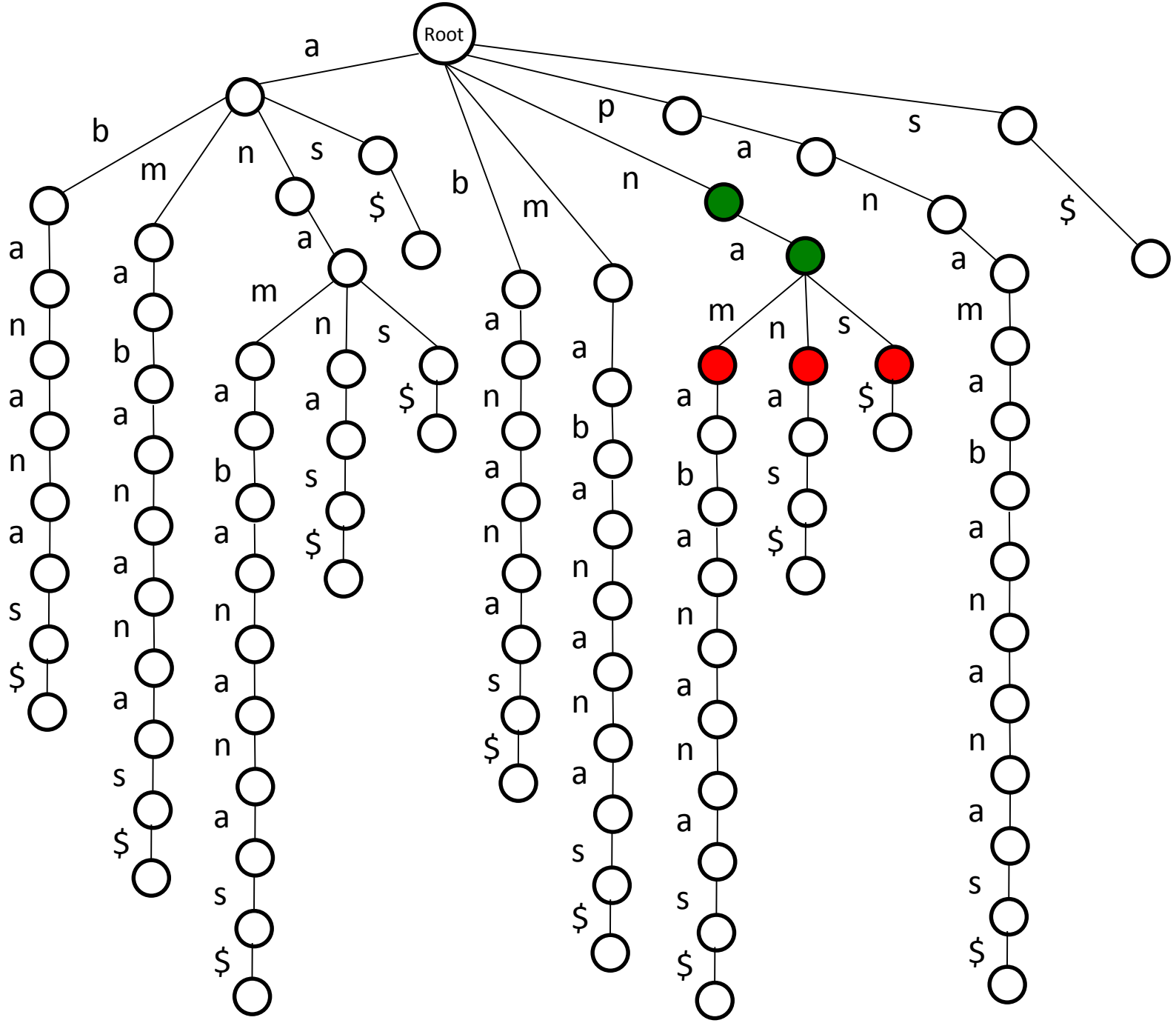
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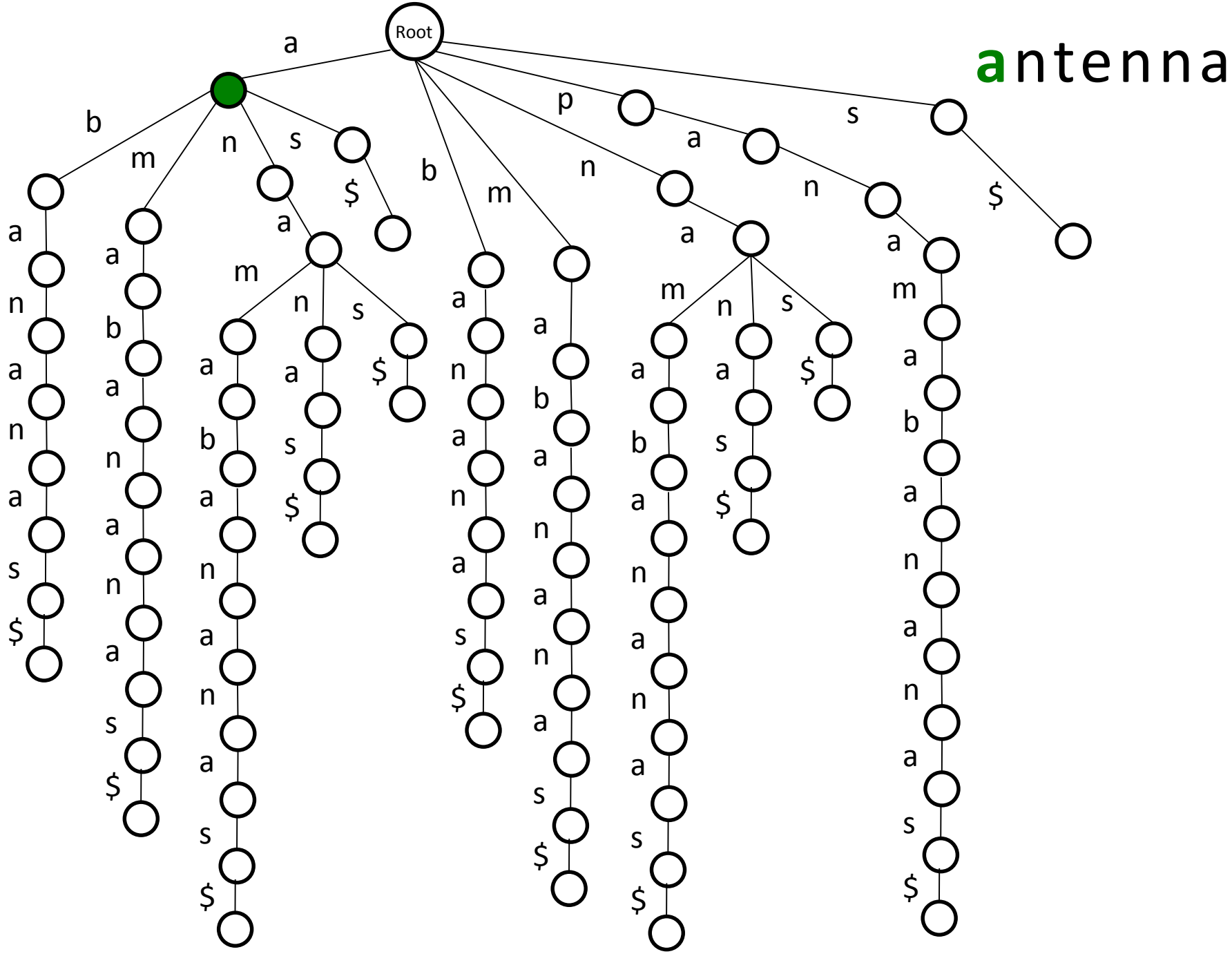
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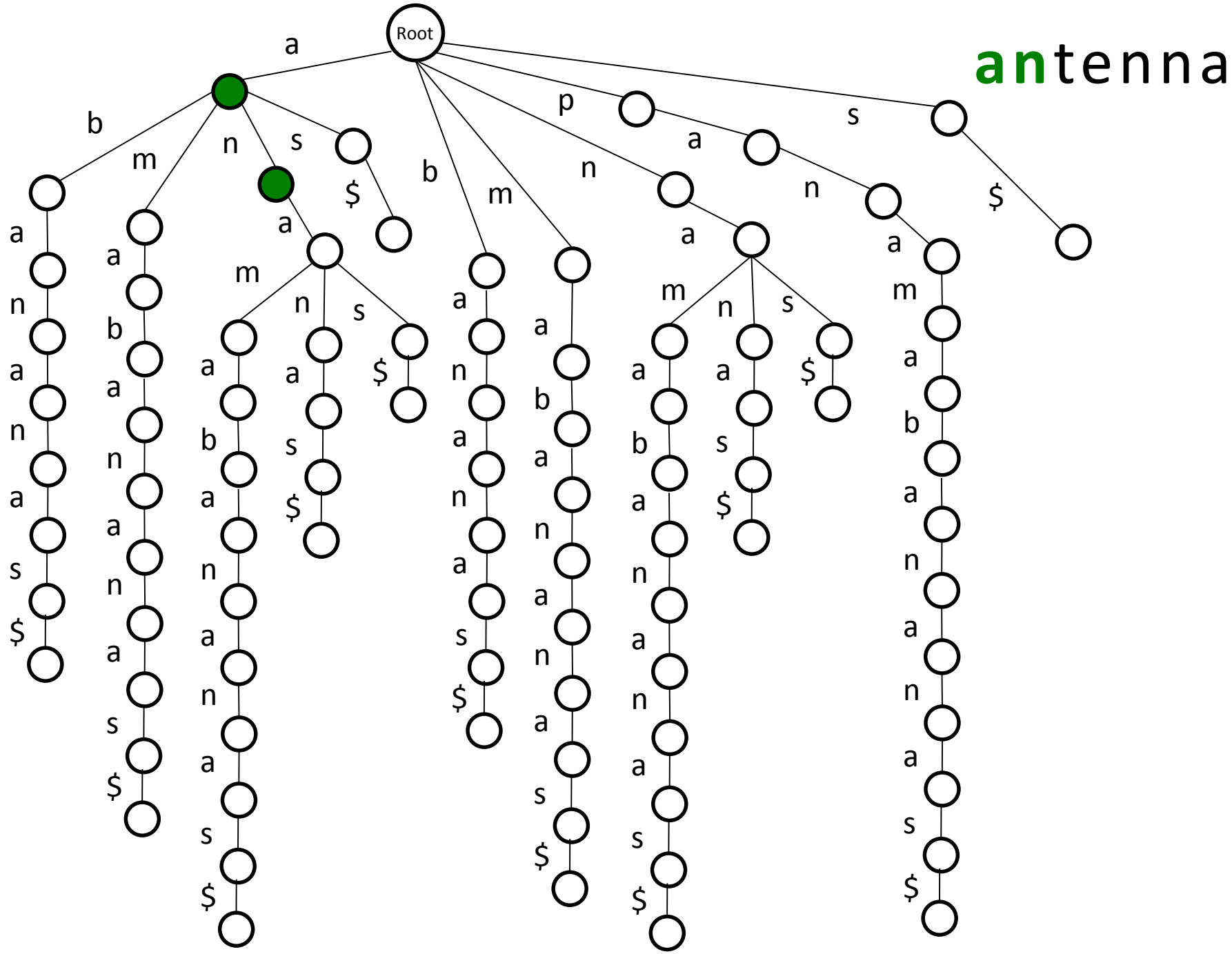
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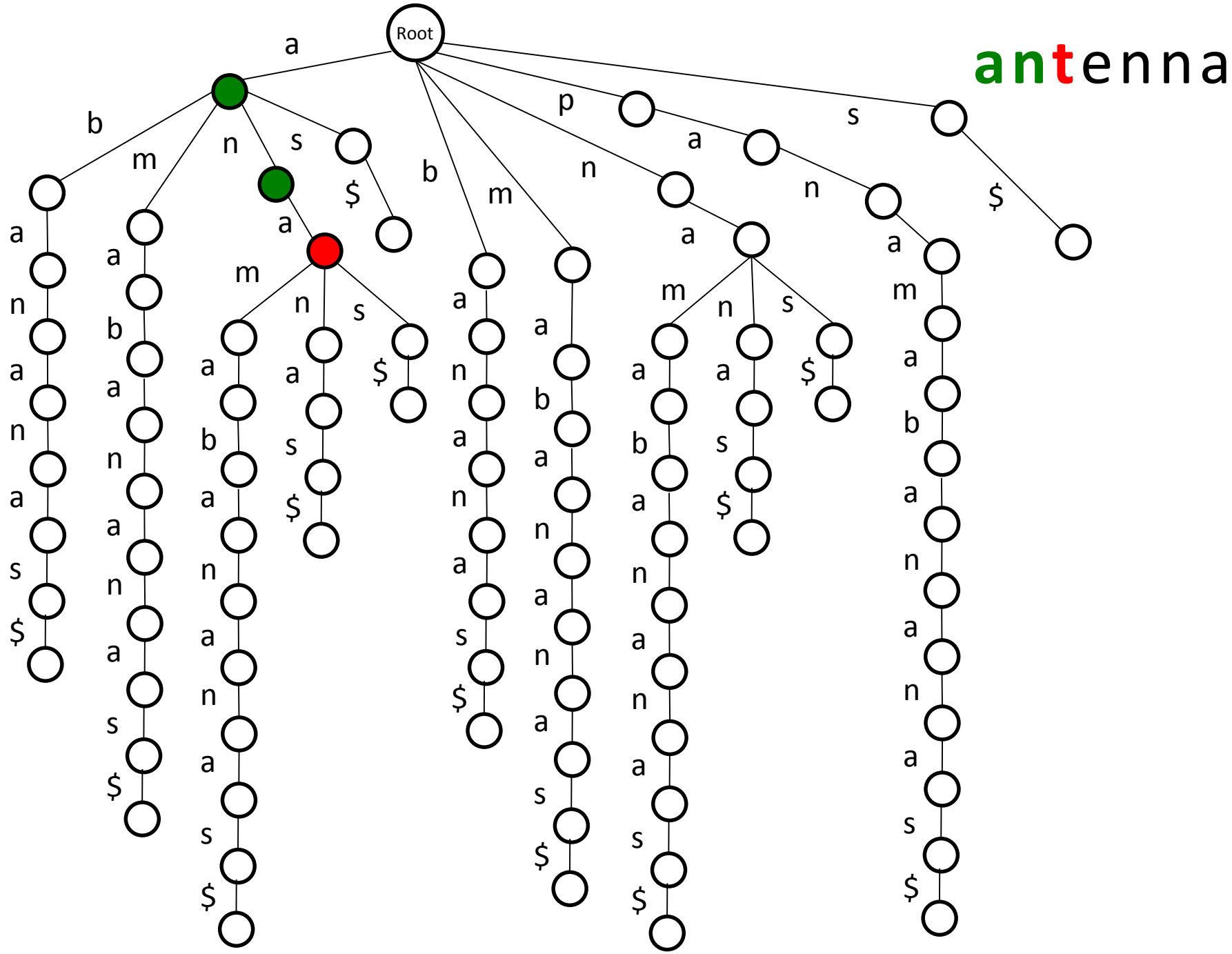
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Where Are the Matches???

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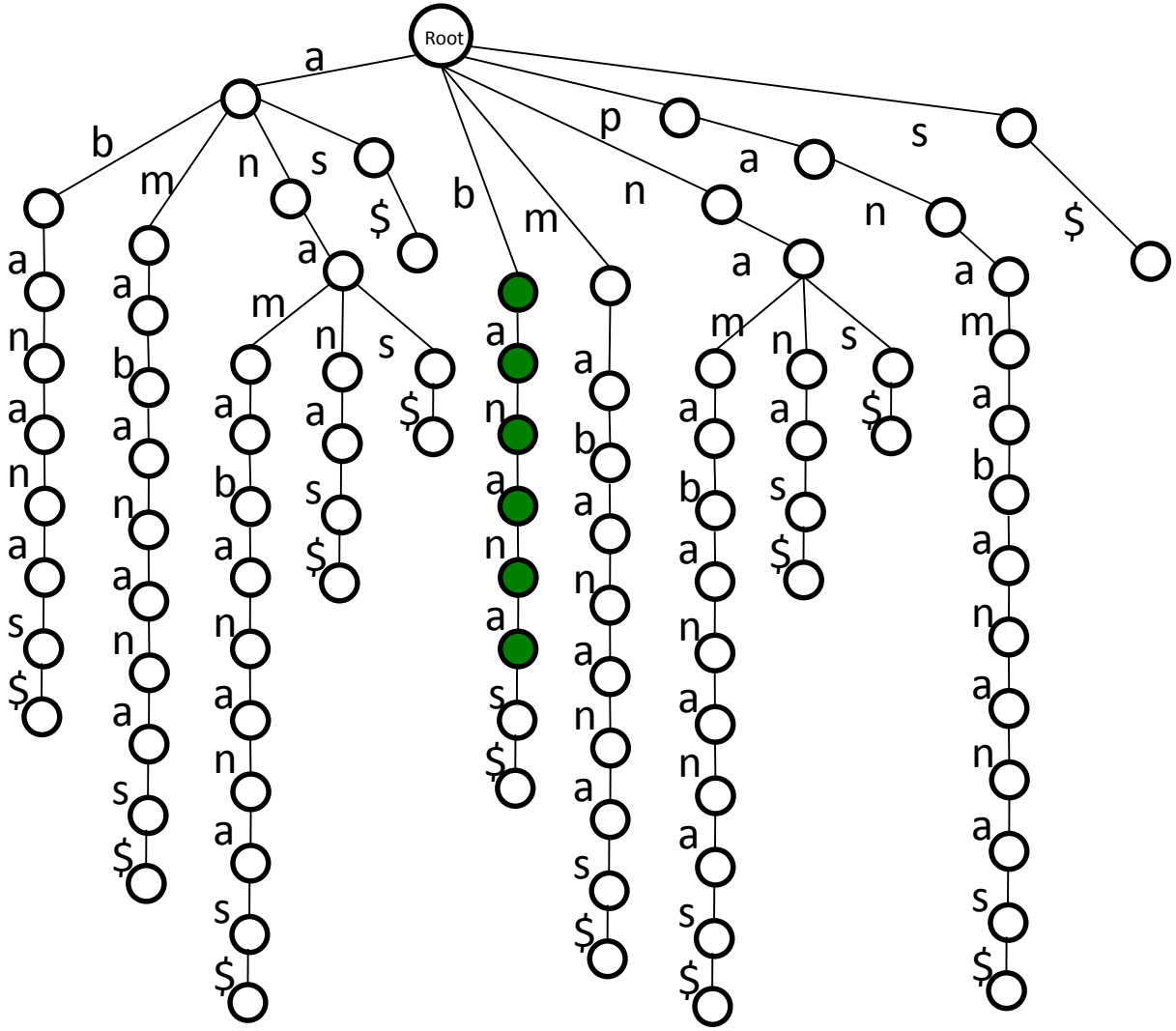
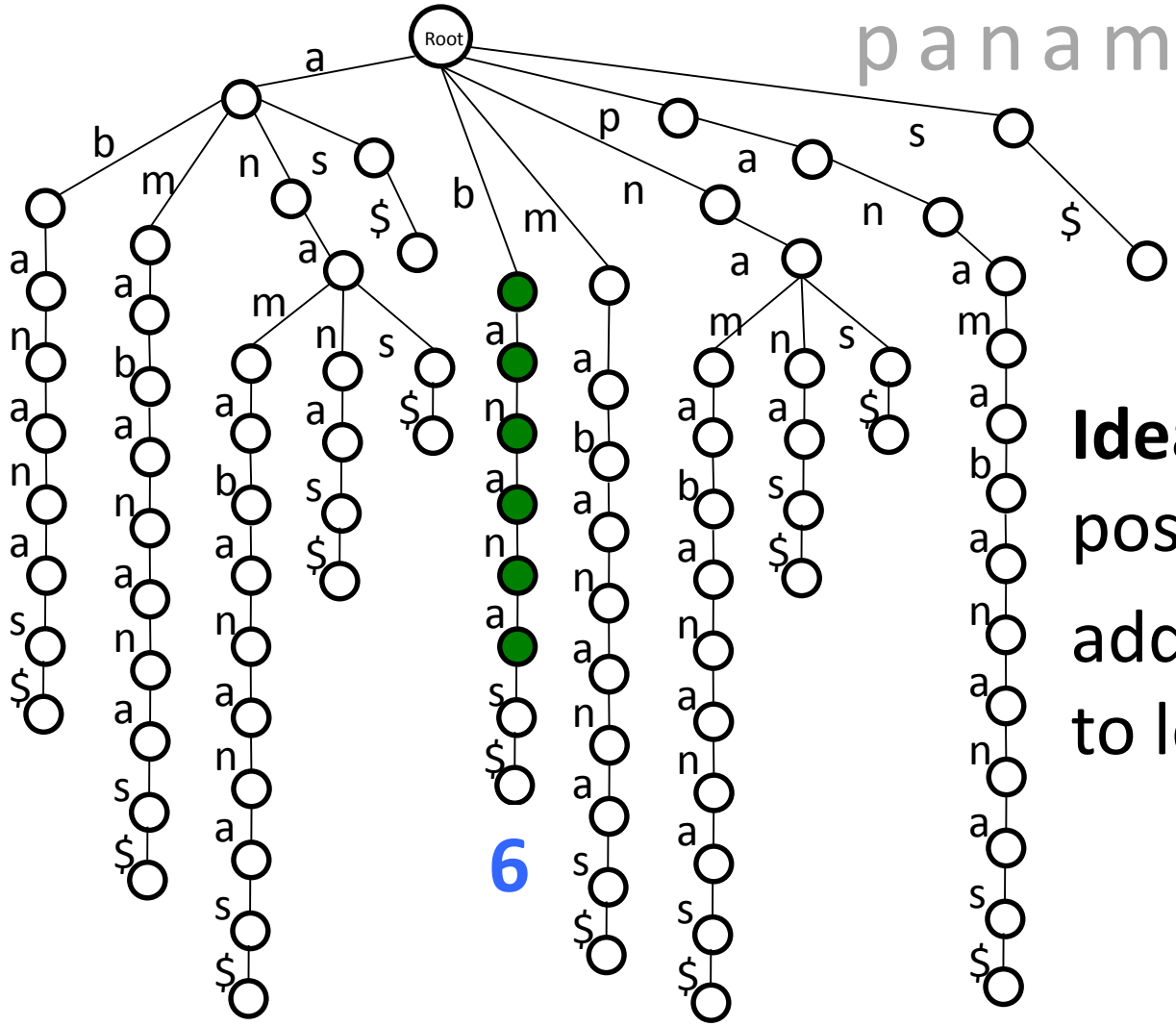


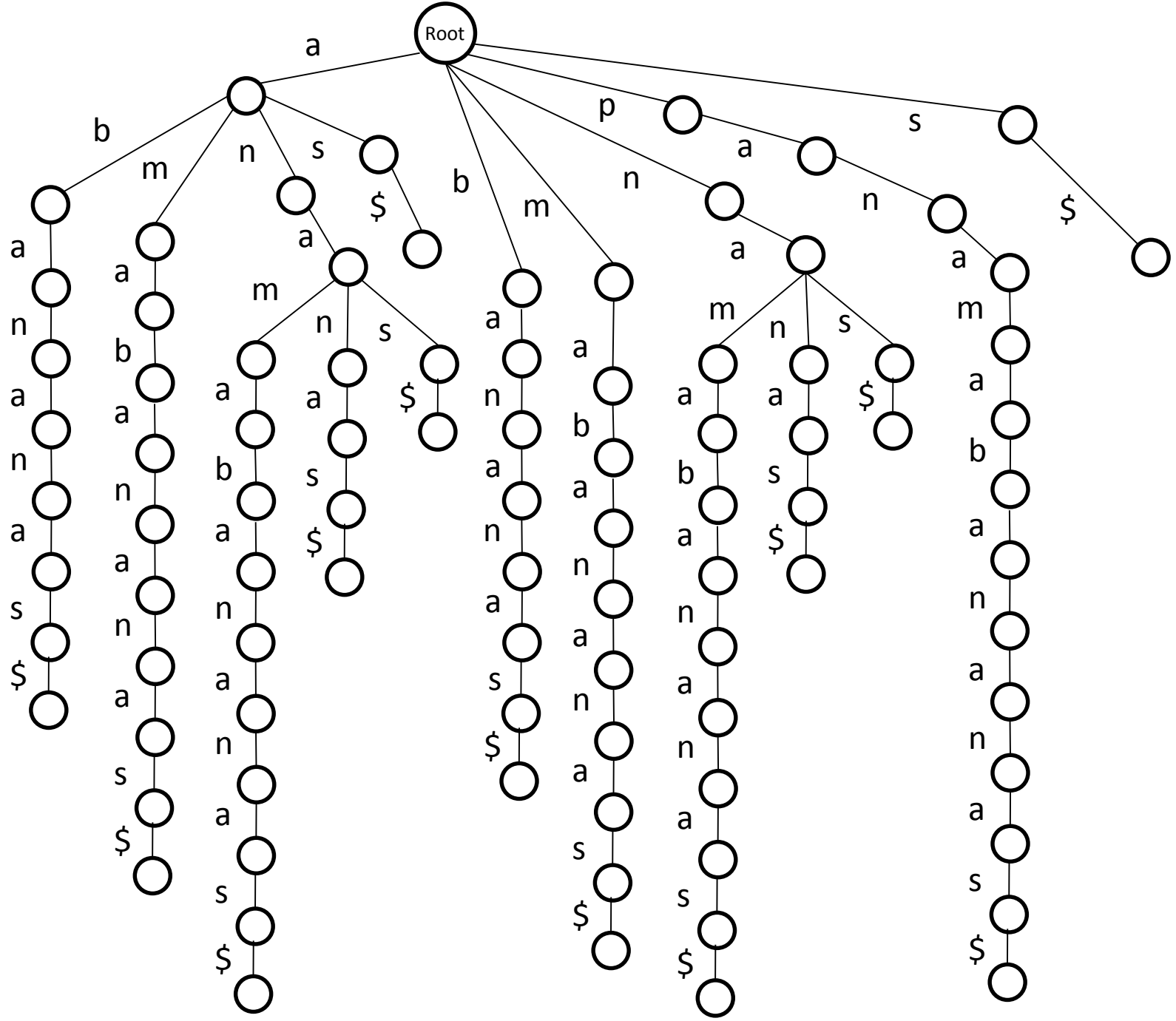
Where Are the Matches???



p a n a m a **b a n a n a s $**

Idea: to find the positions of matches,

add some information to leaves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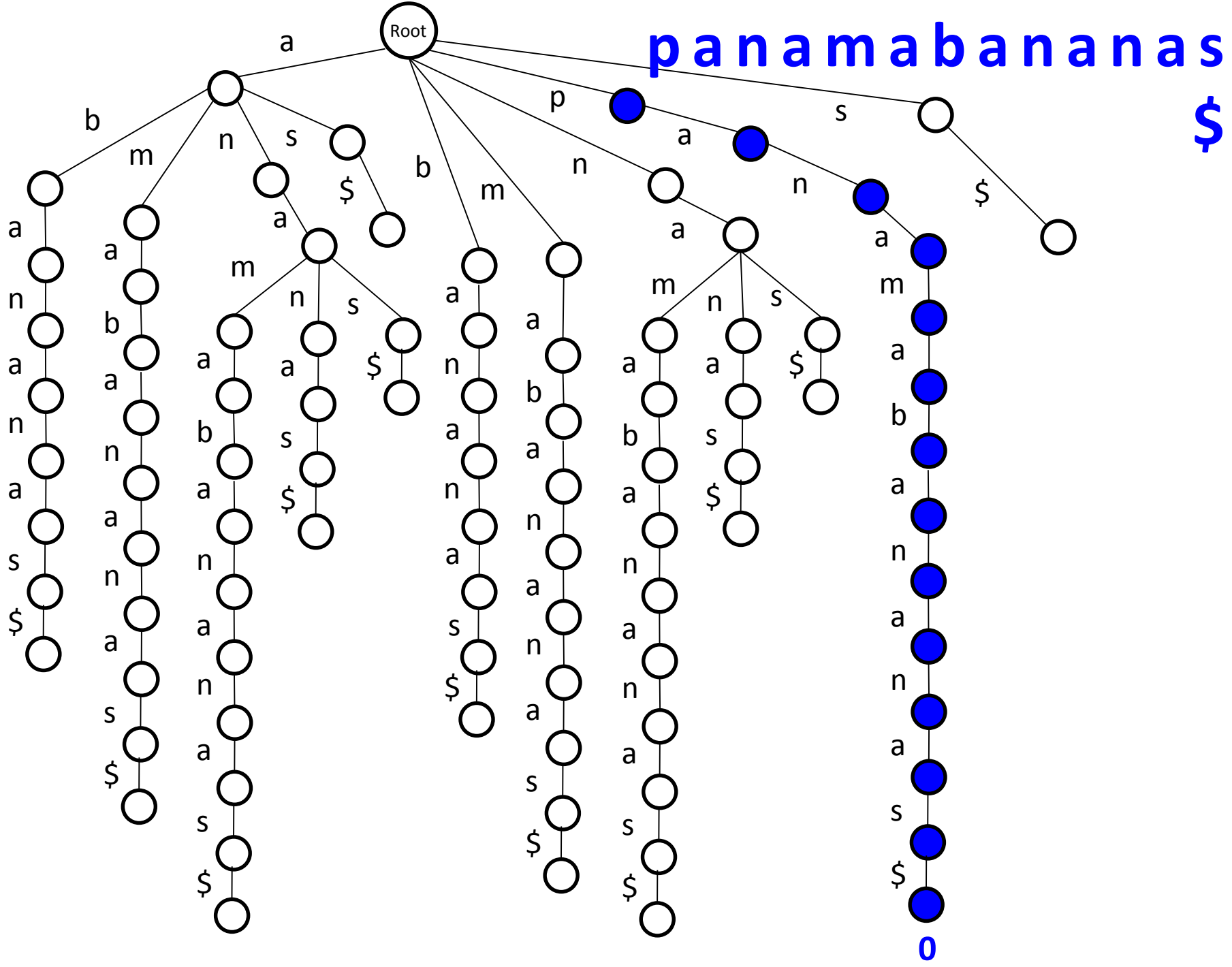
Root
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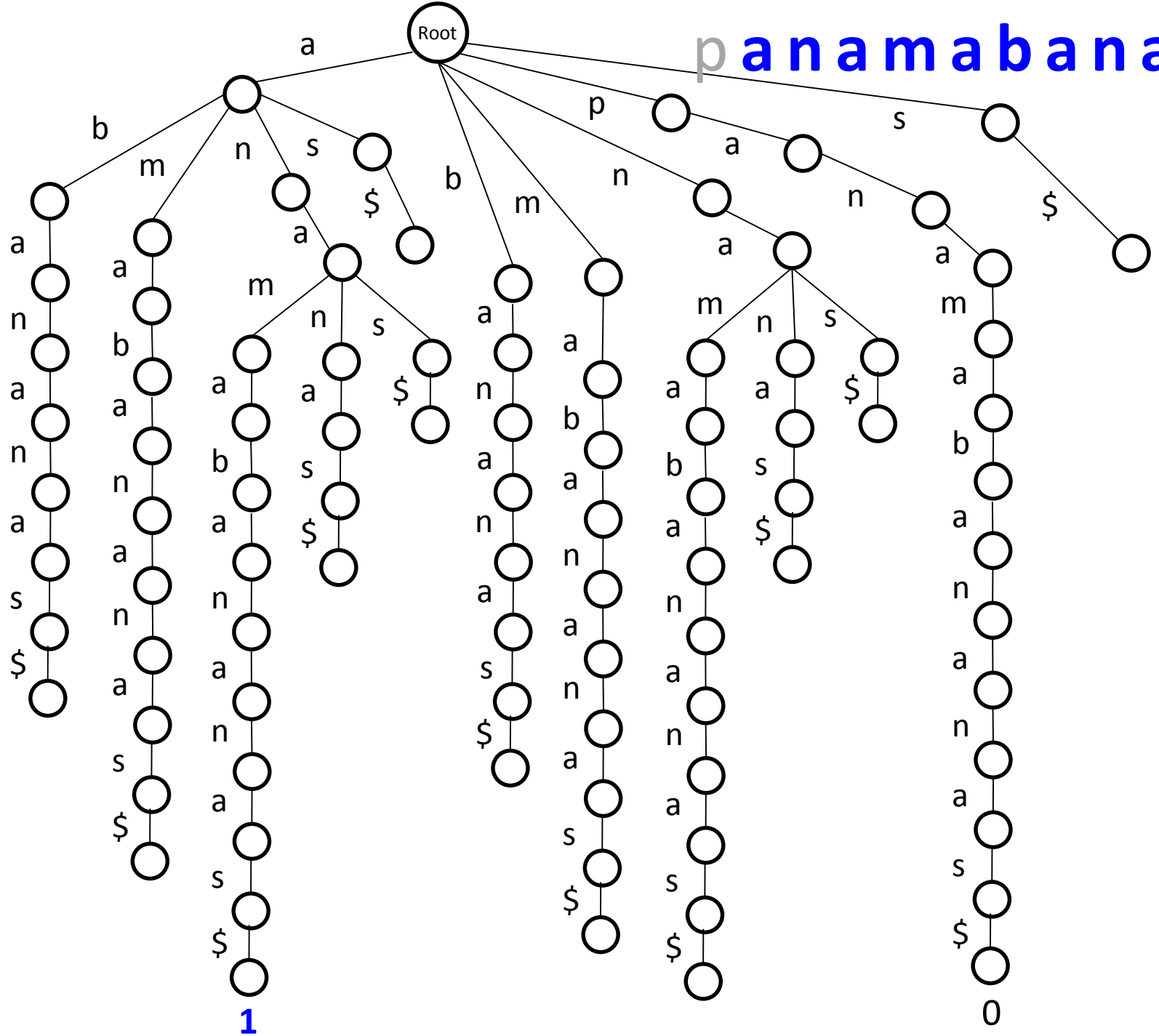
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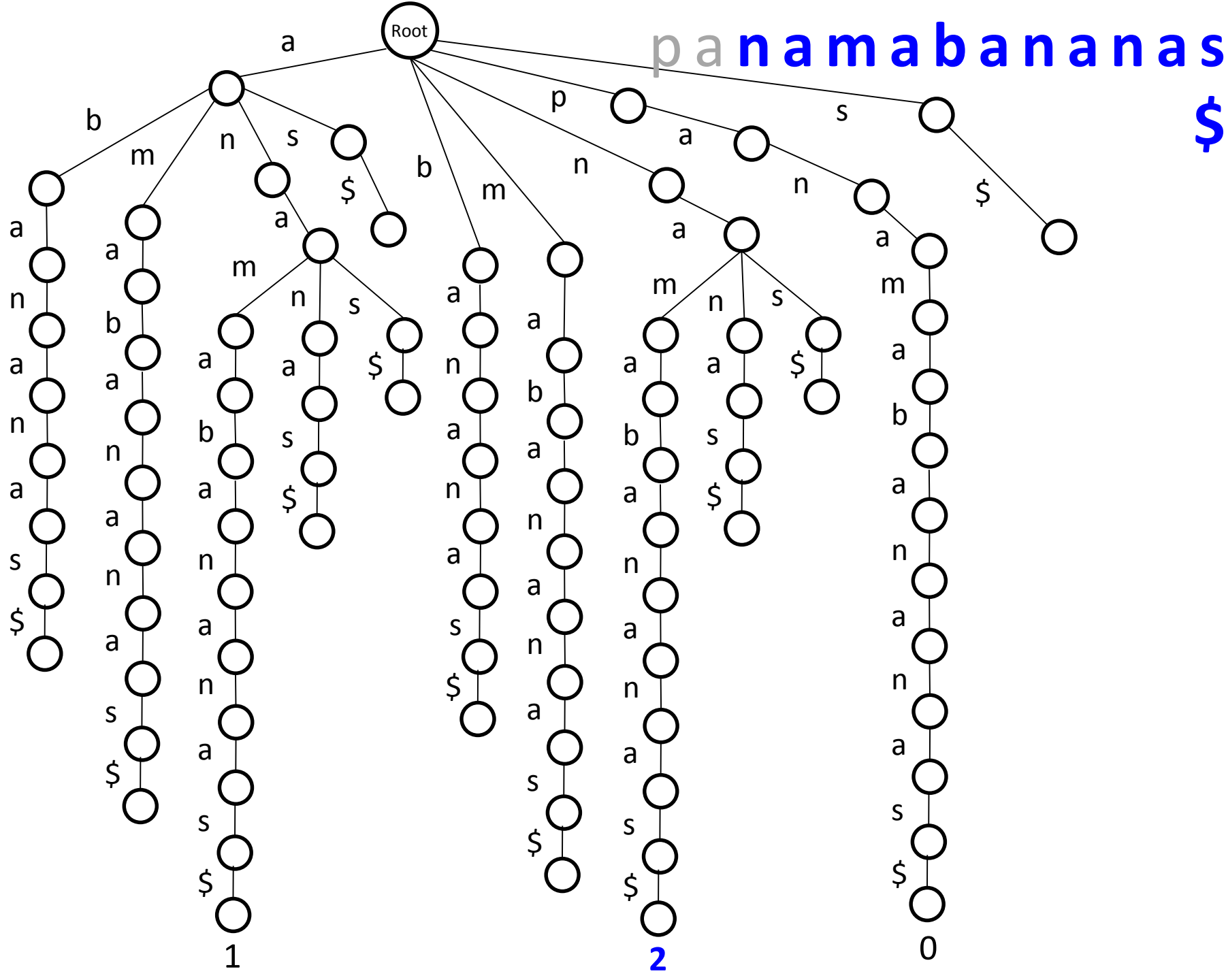
Root
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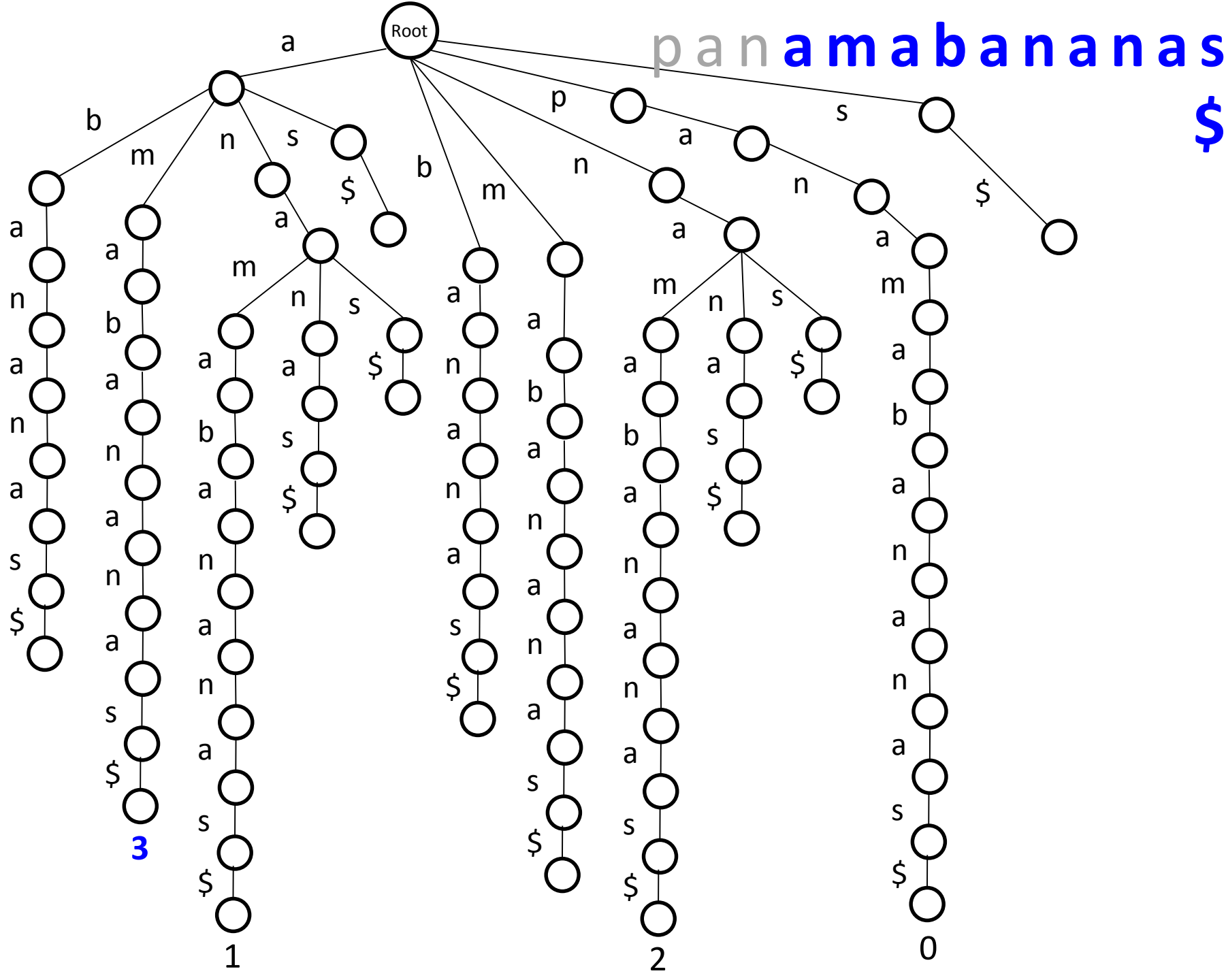
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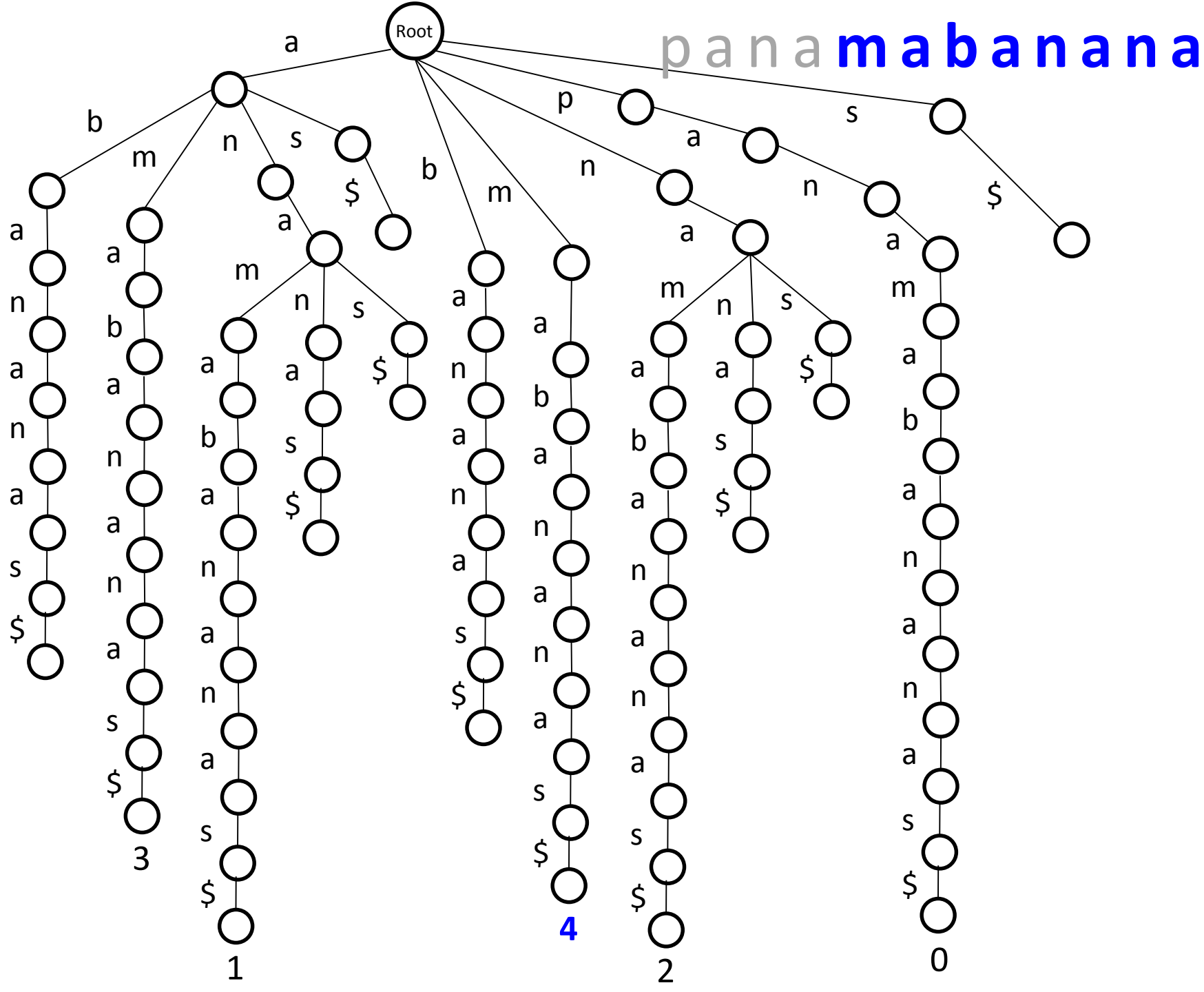
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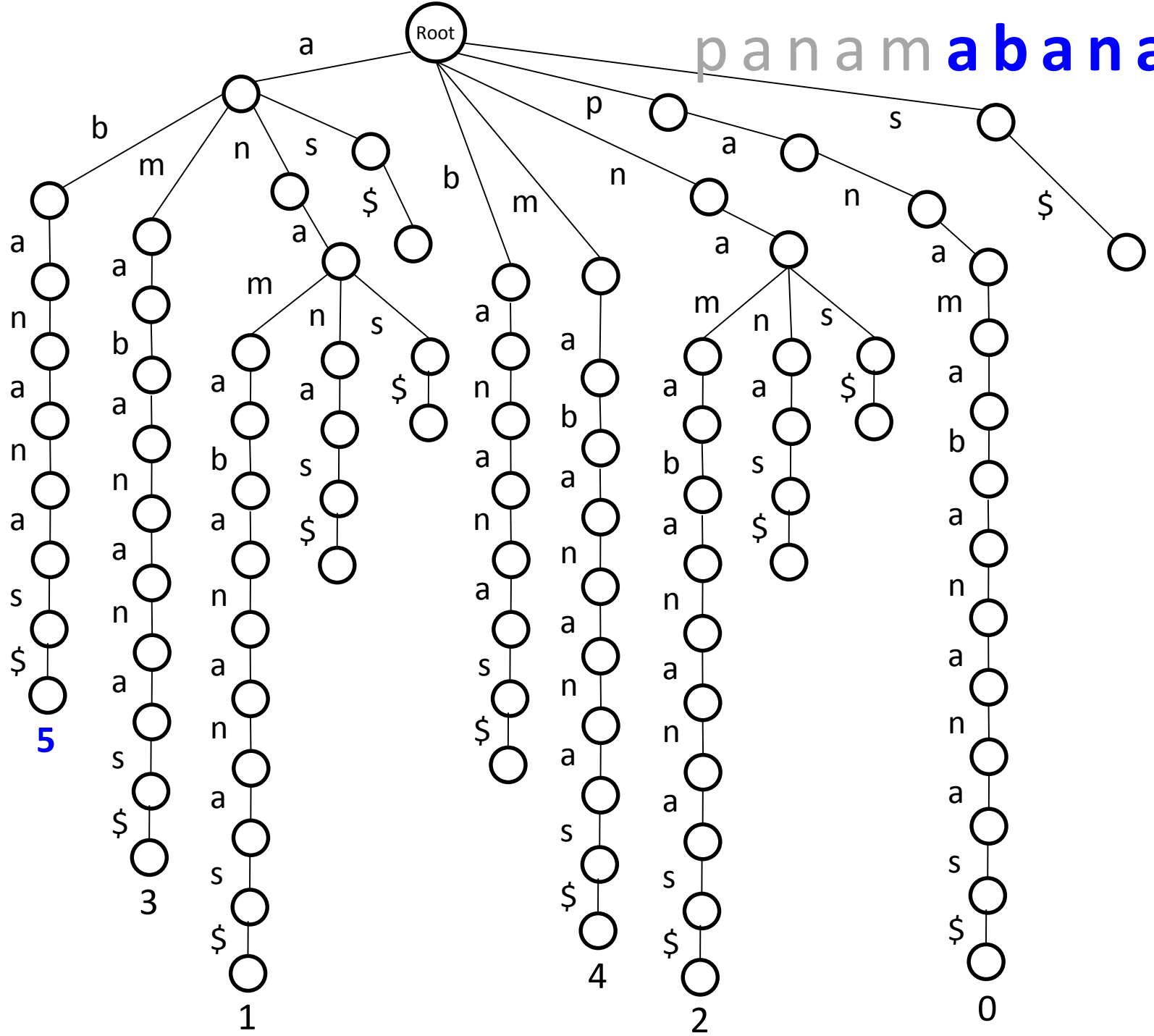
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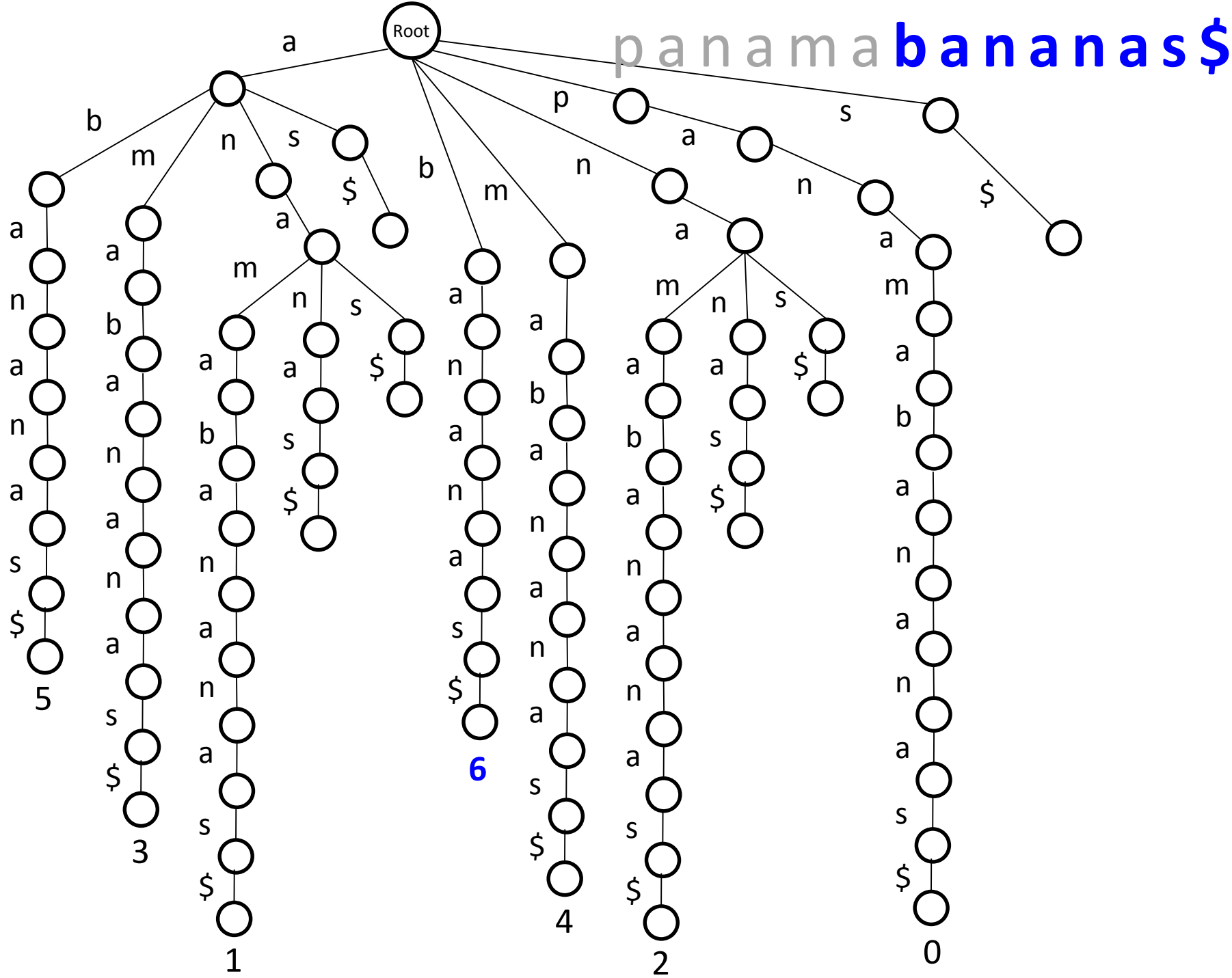
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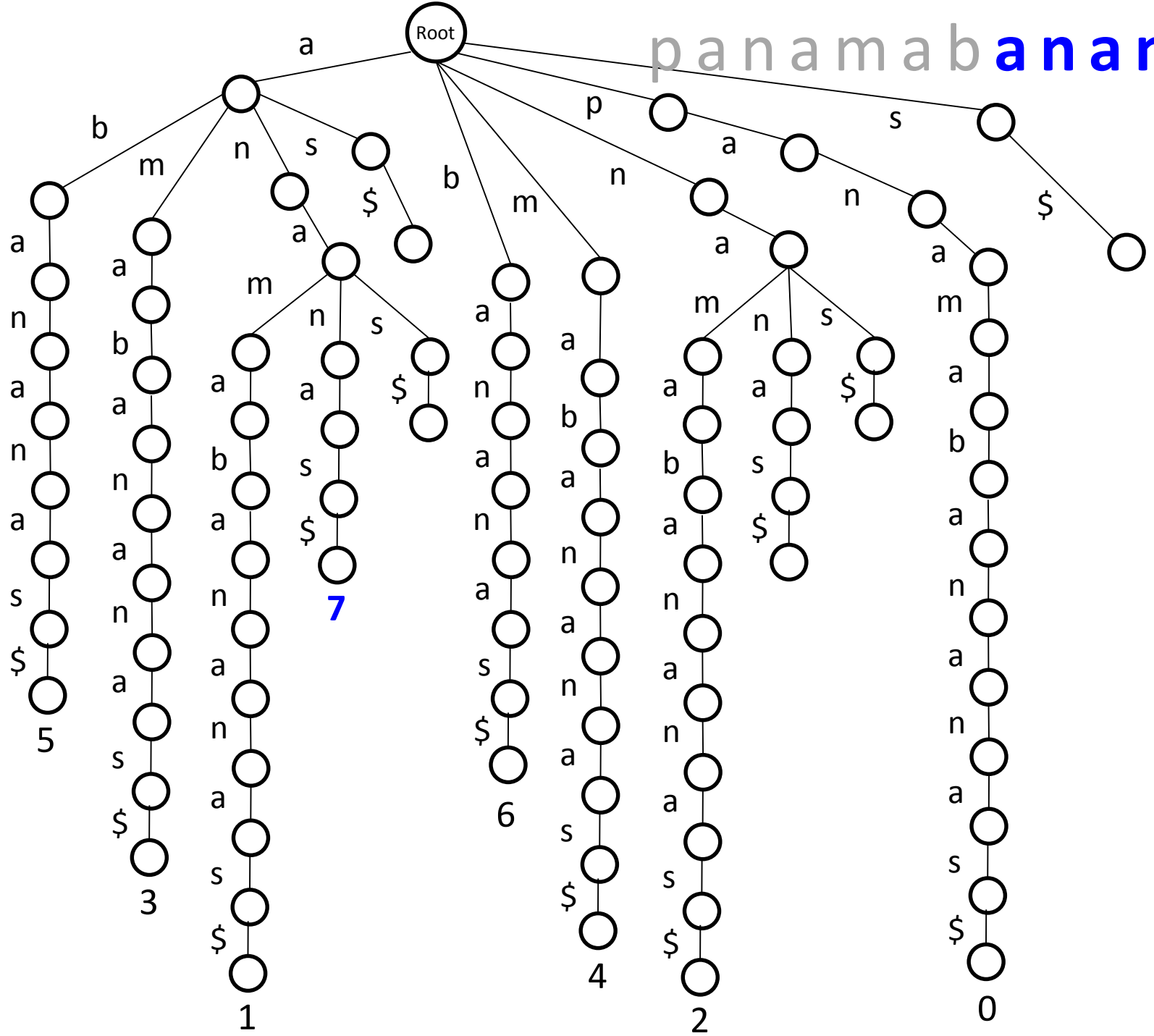
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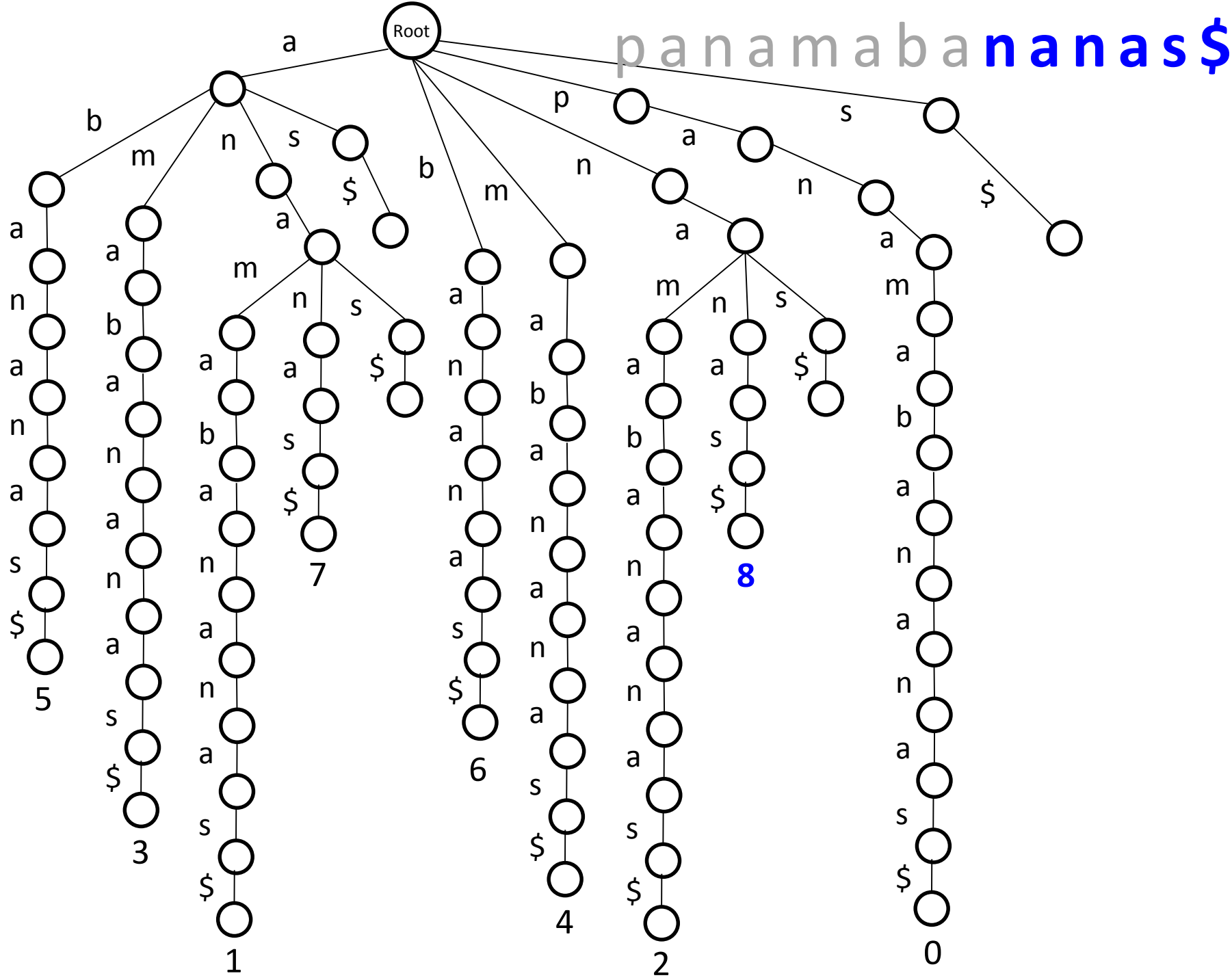
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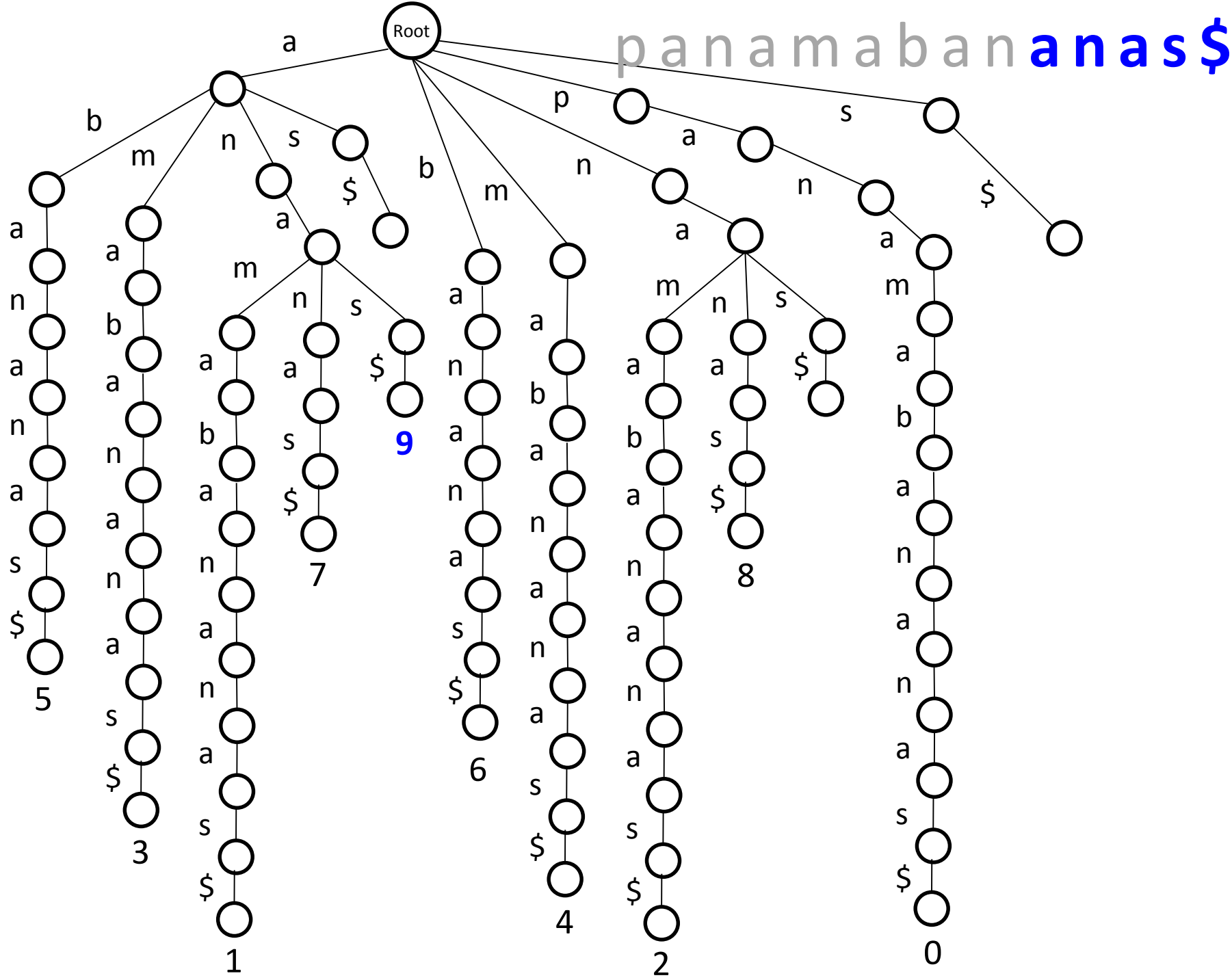
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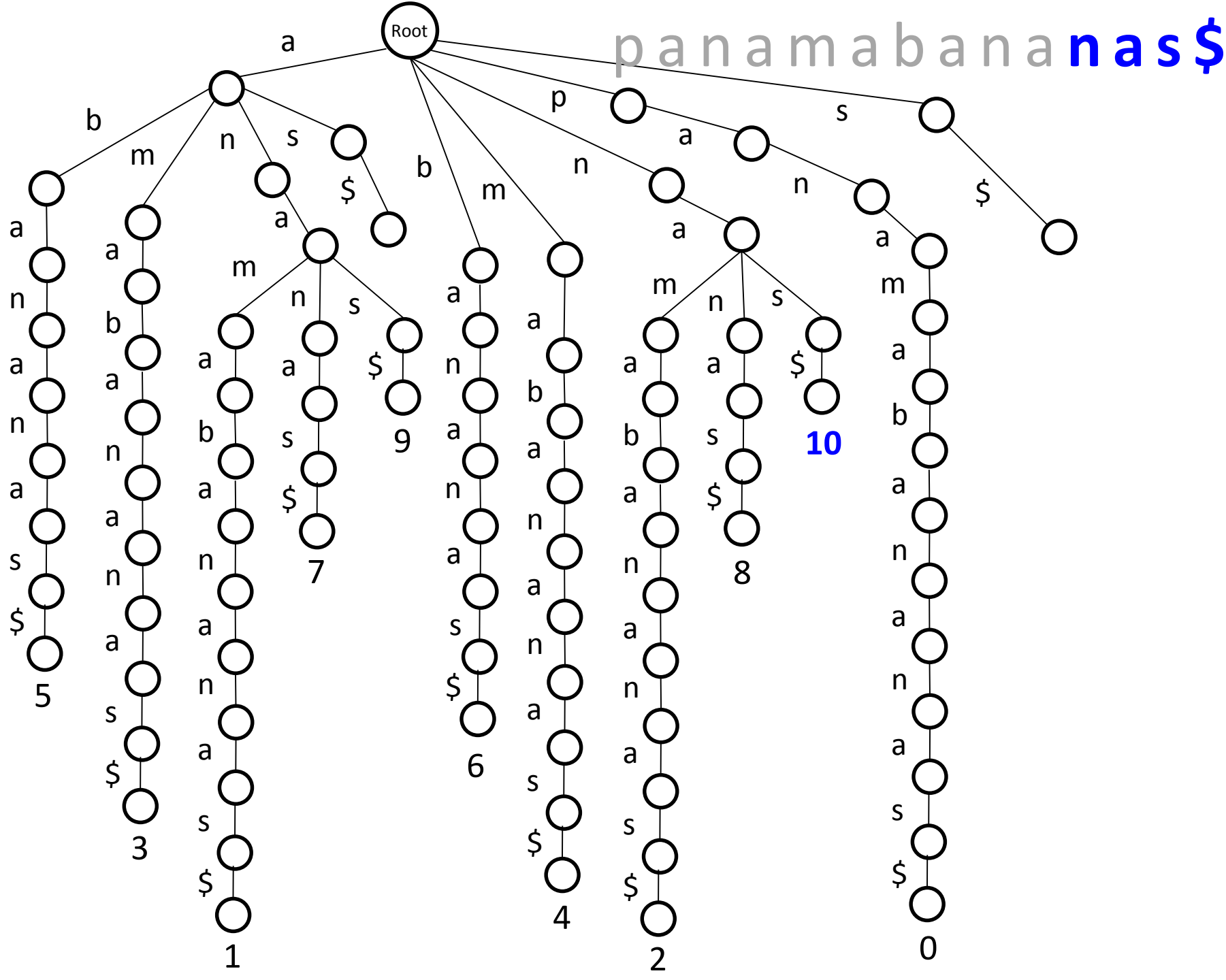
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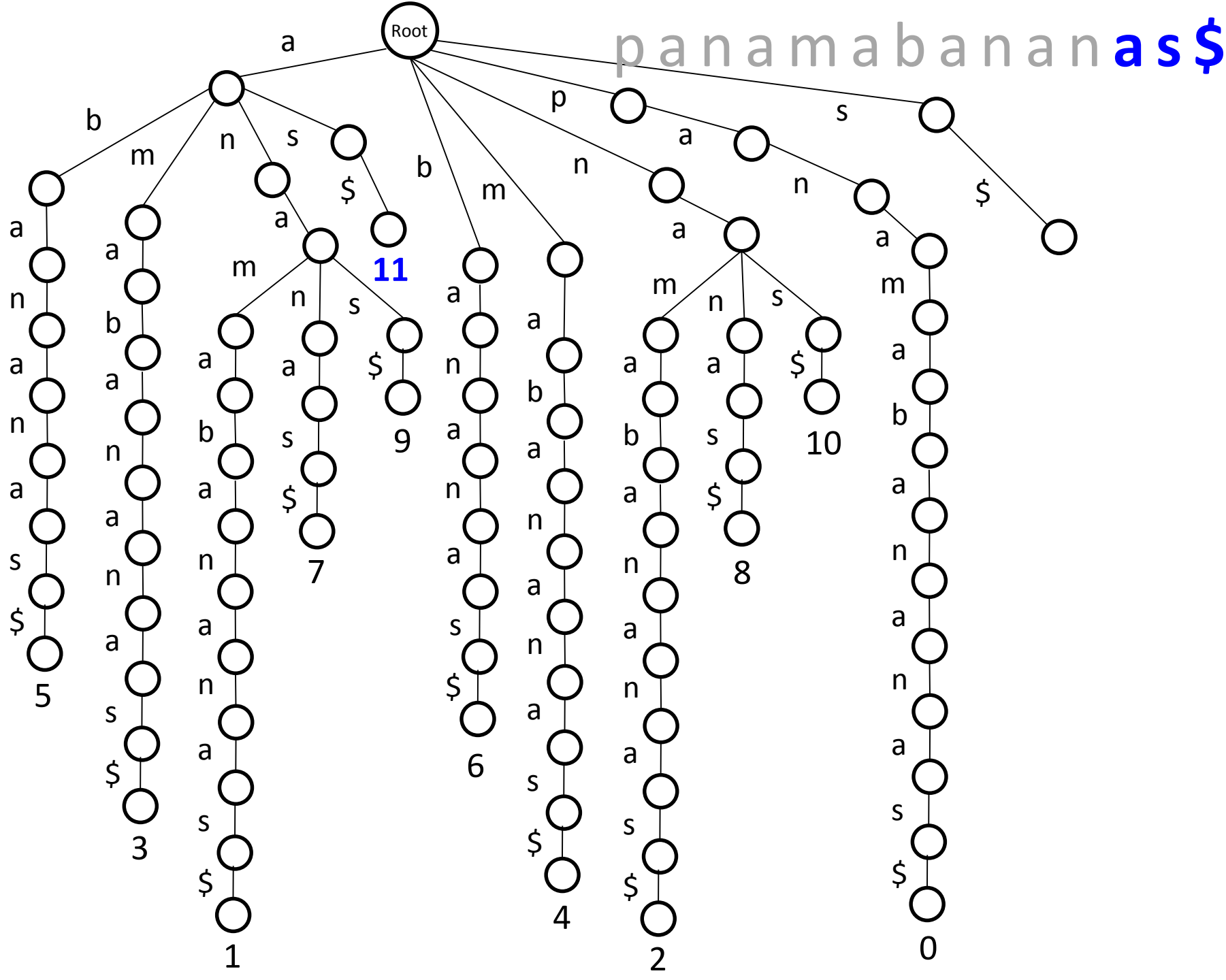
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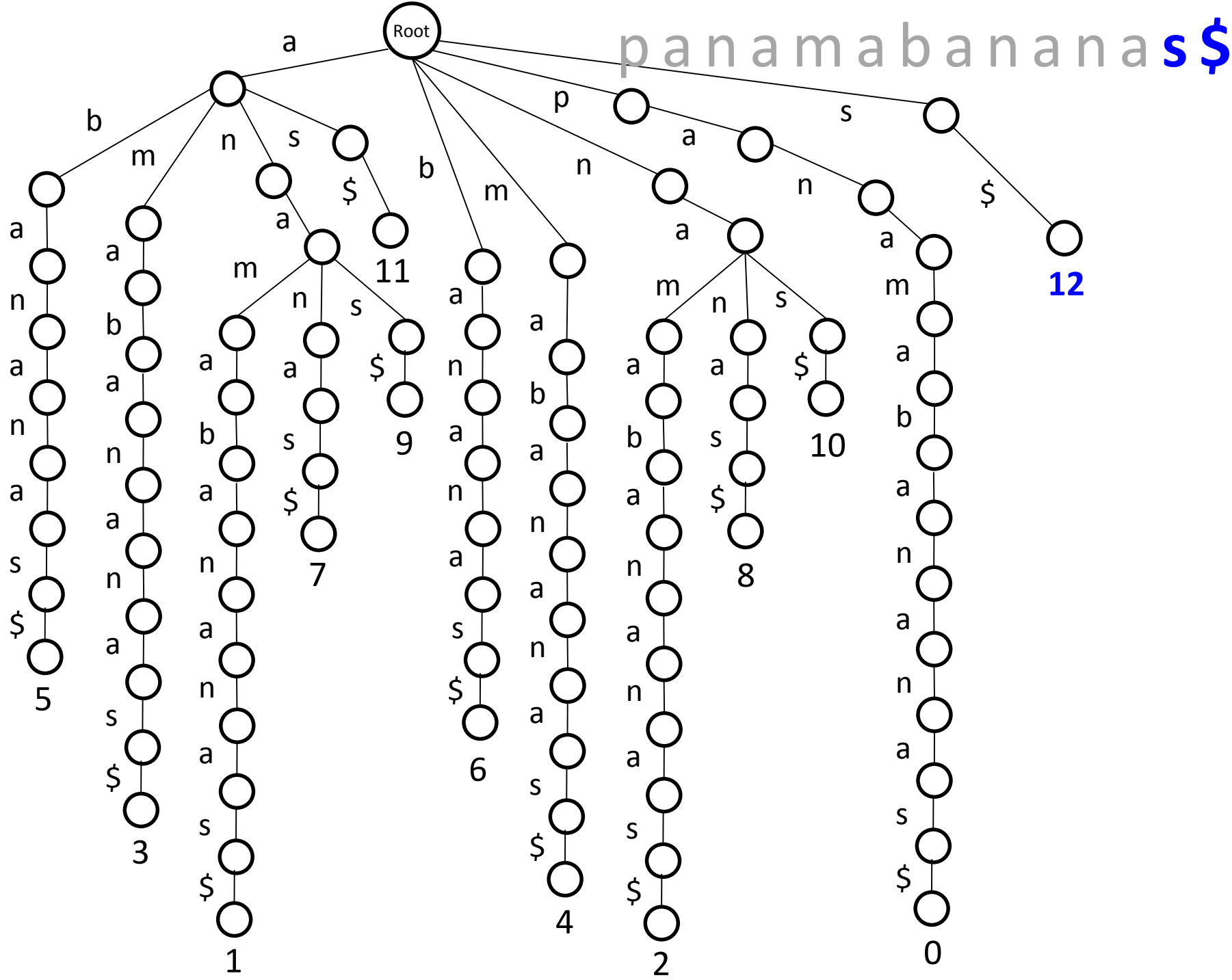
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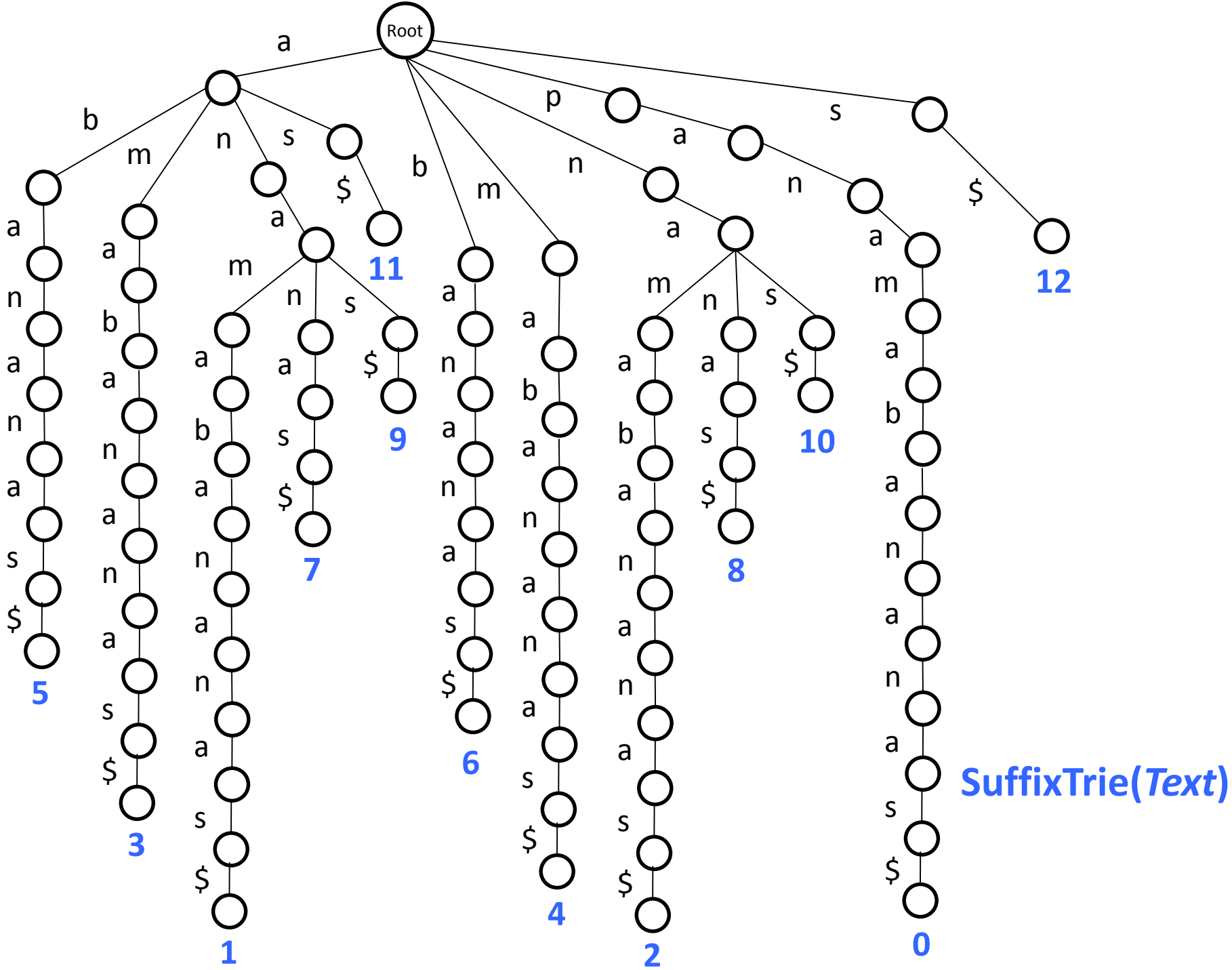
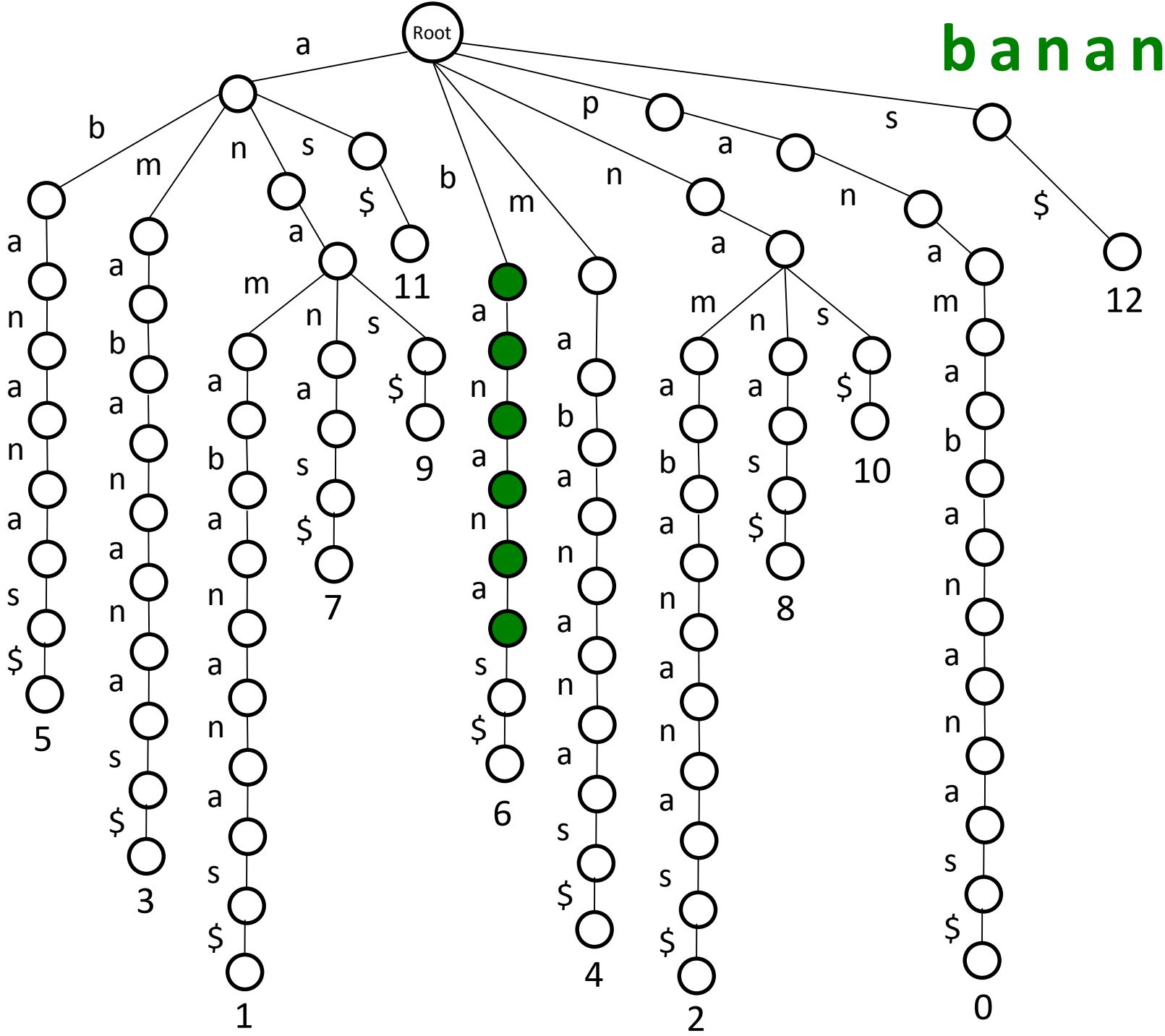

Root
SuffixTrie(*Text*)

Walking Down to the Leaves to Find Matches

- Once we find a match, we “walk down” to the leaf (or leaves) in order to find the starting position of the match.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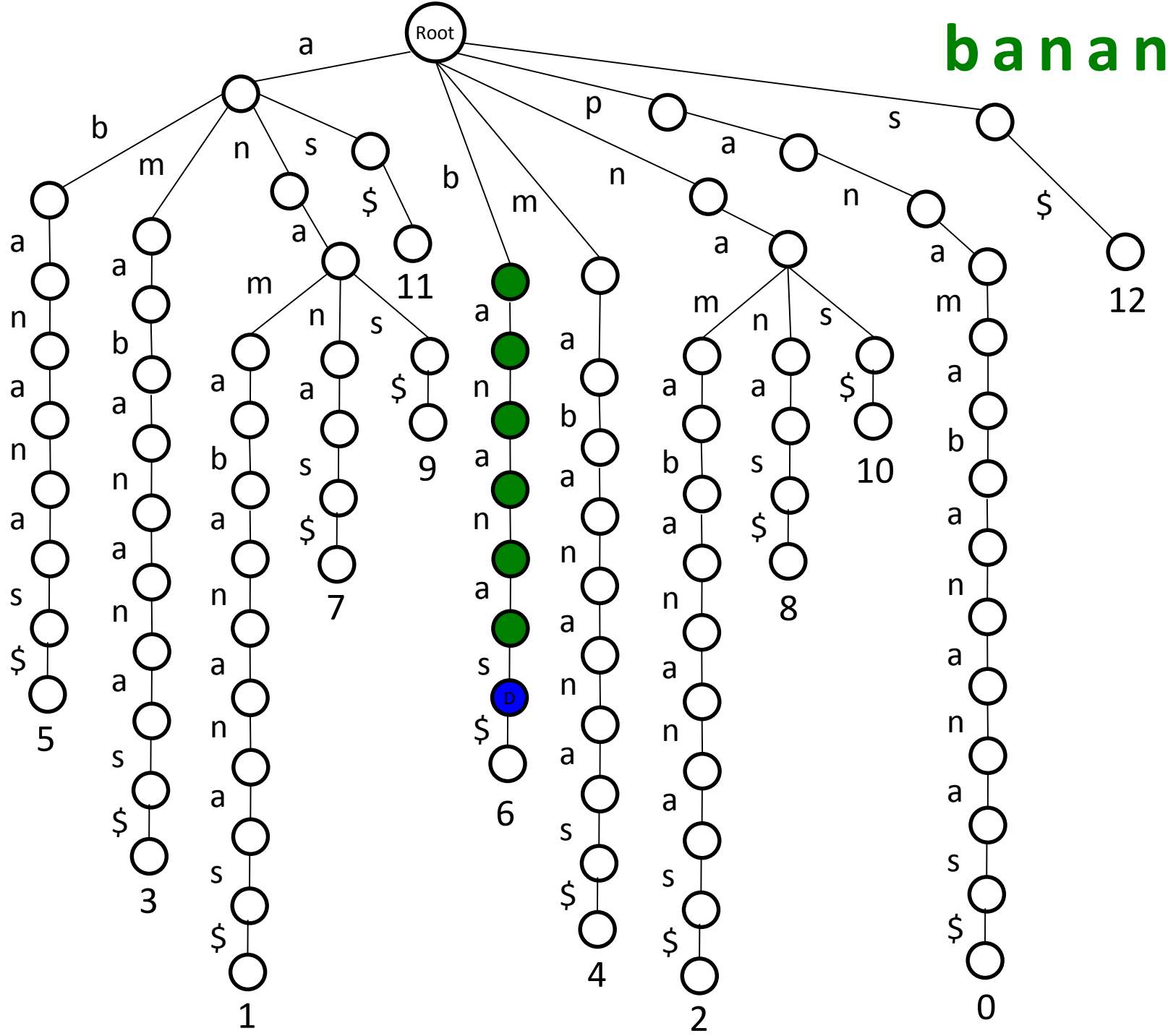
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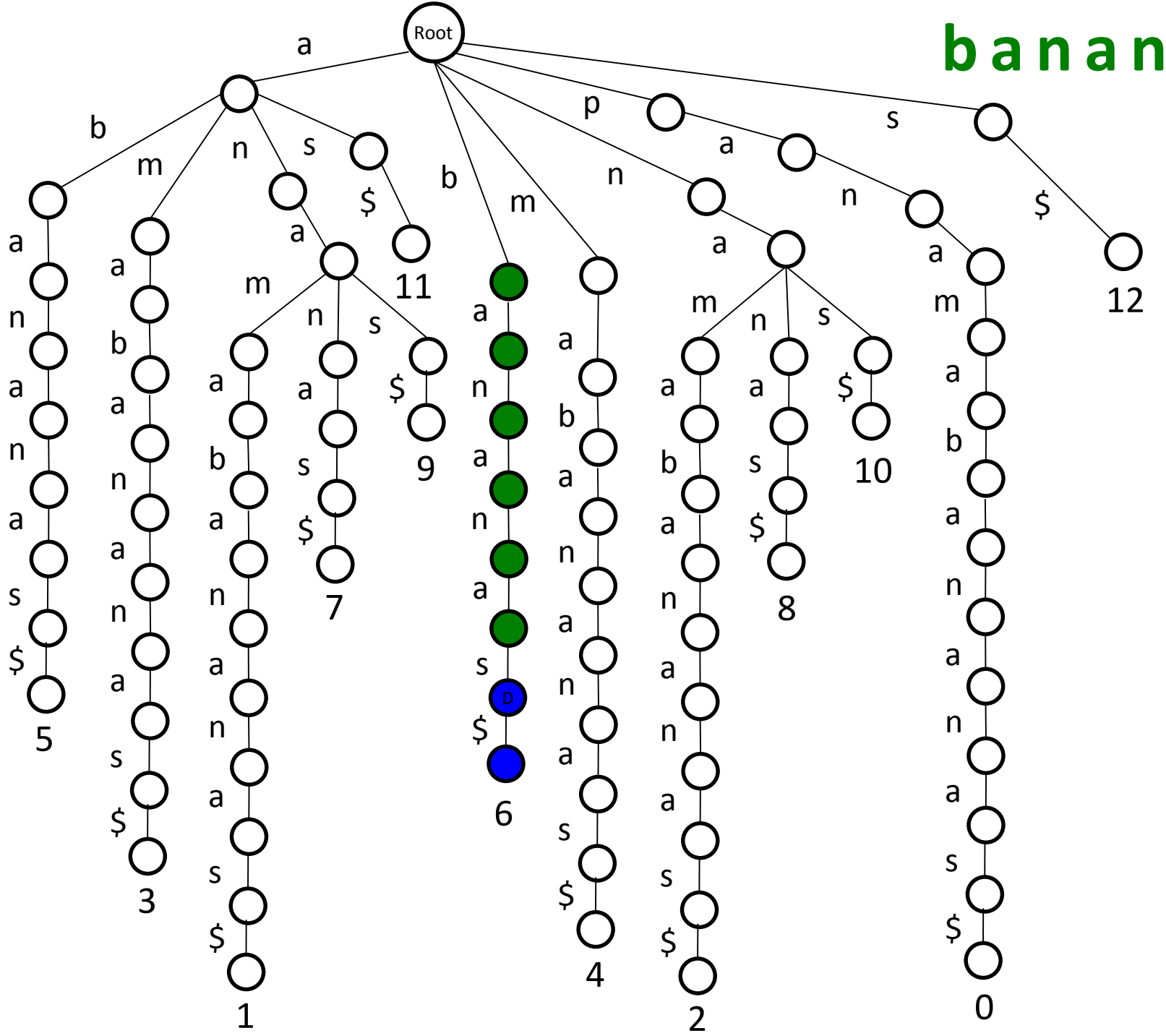
banana
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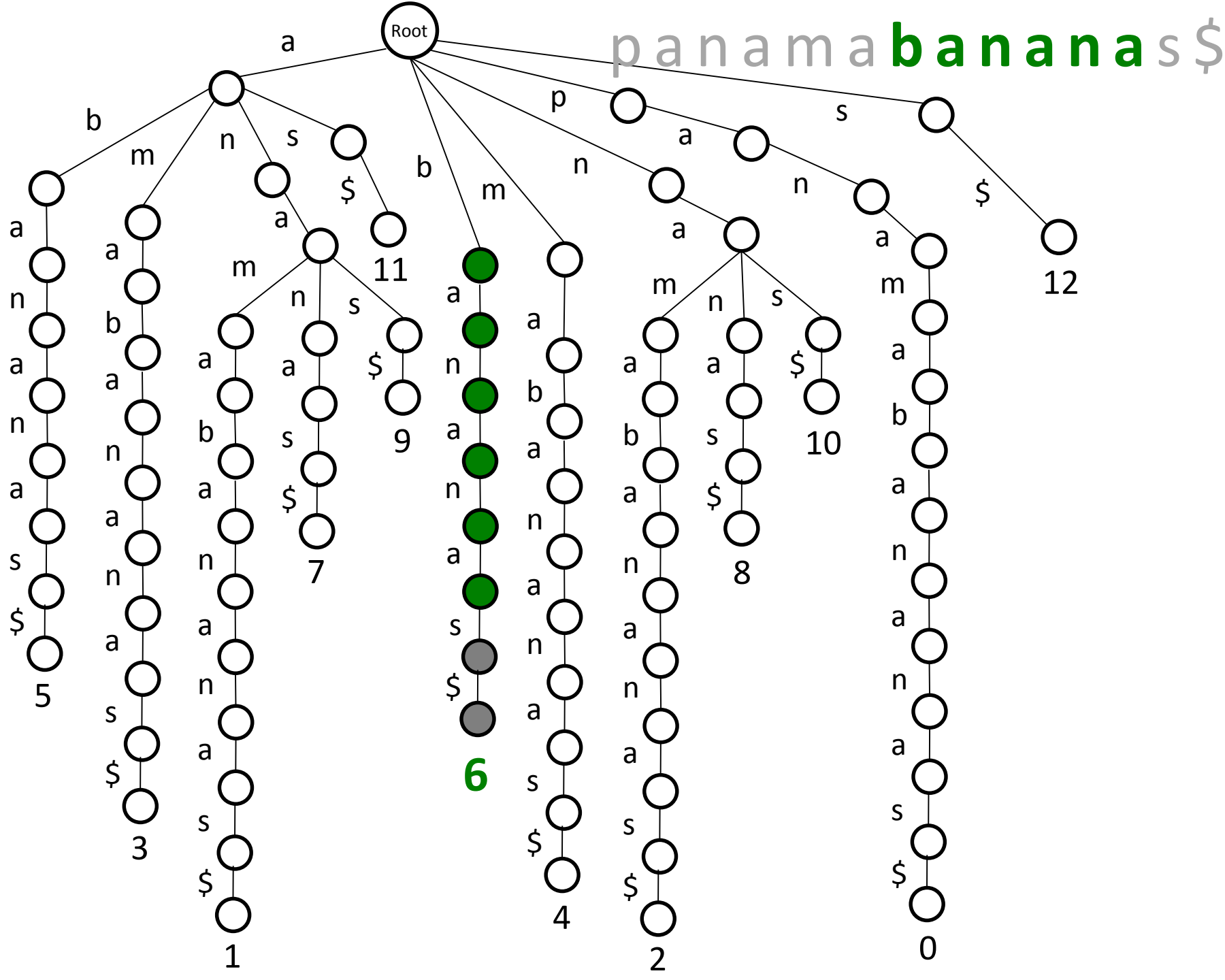
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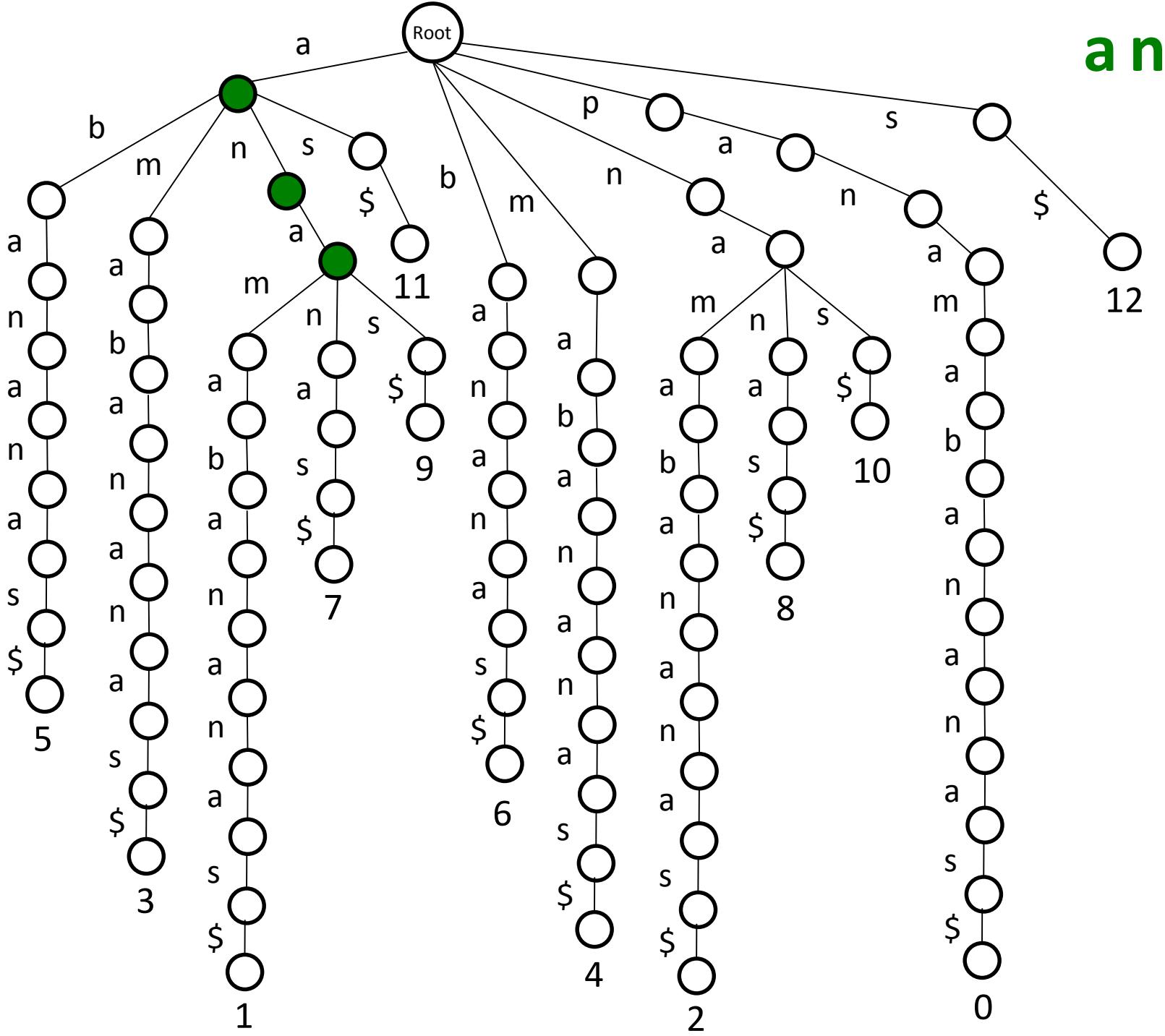
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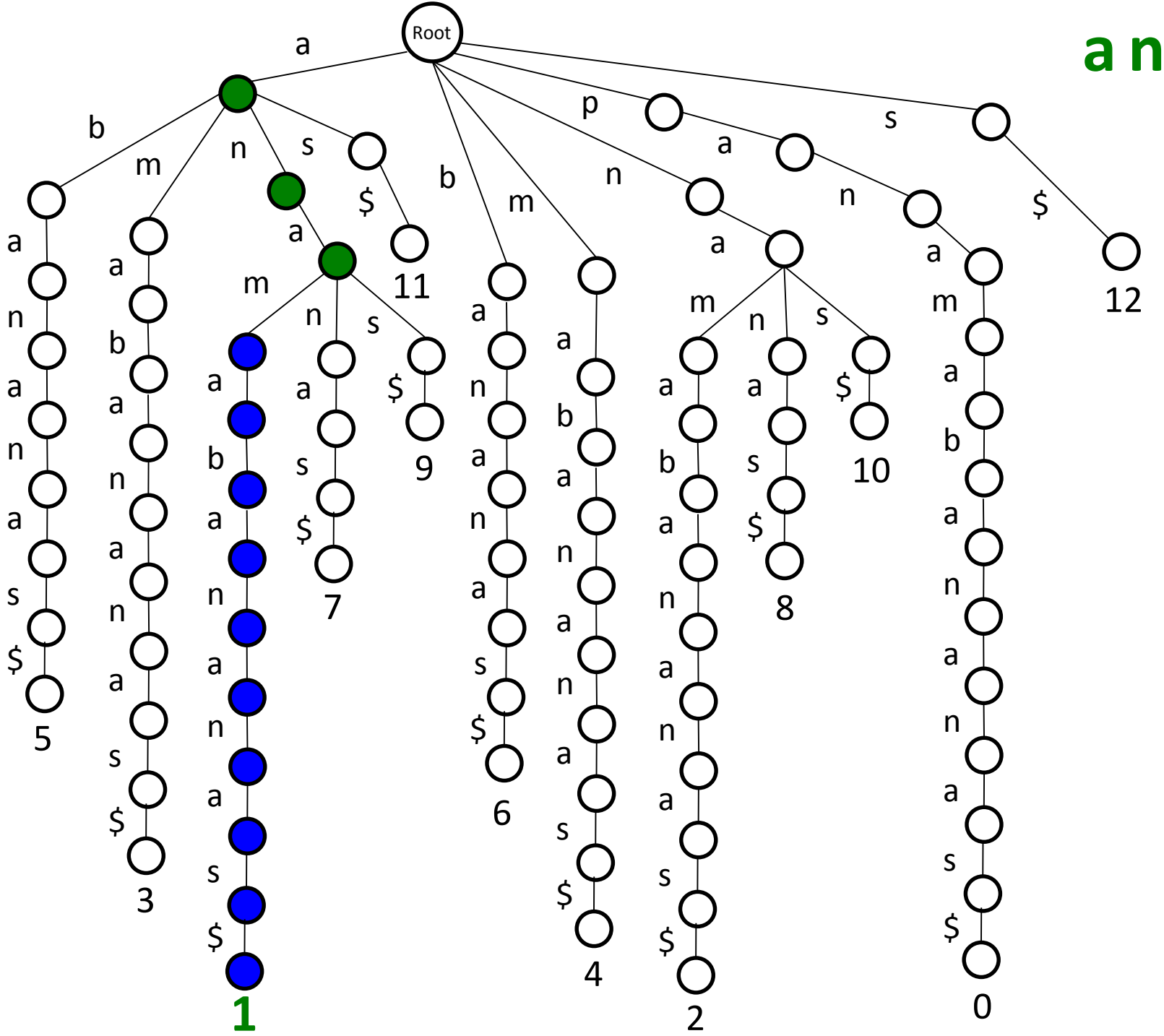
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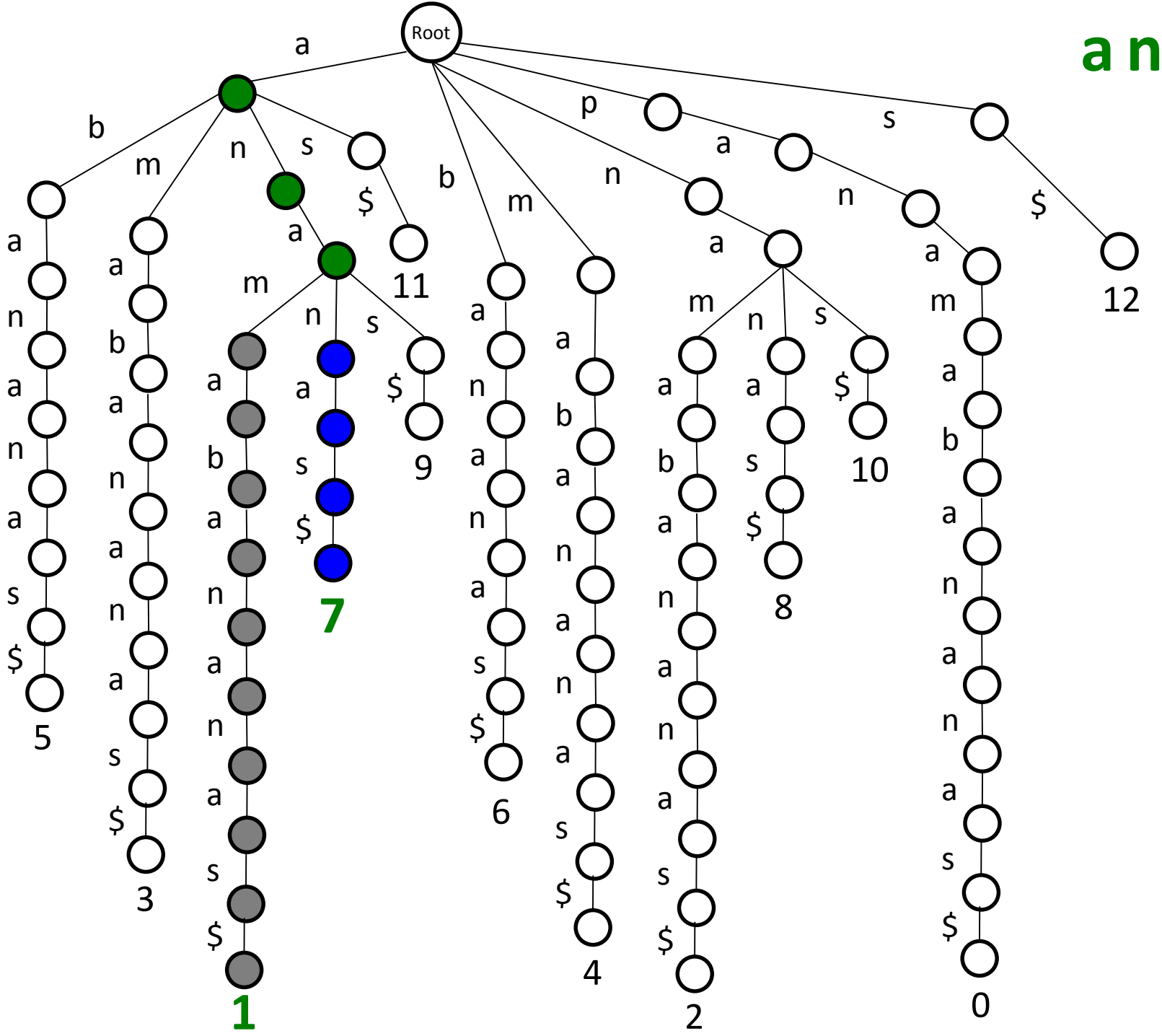
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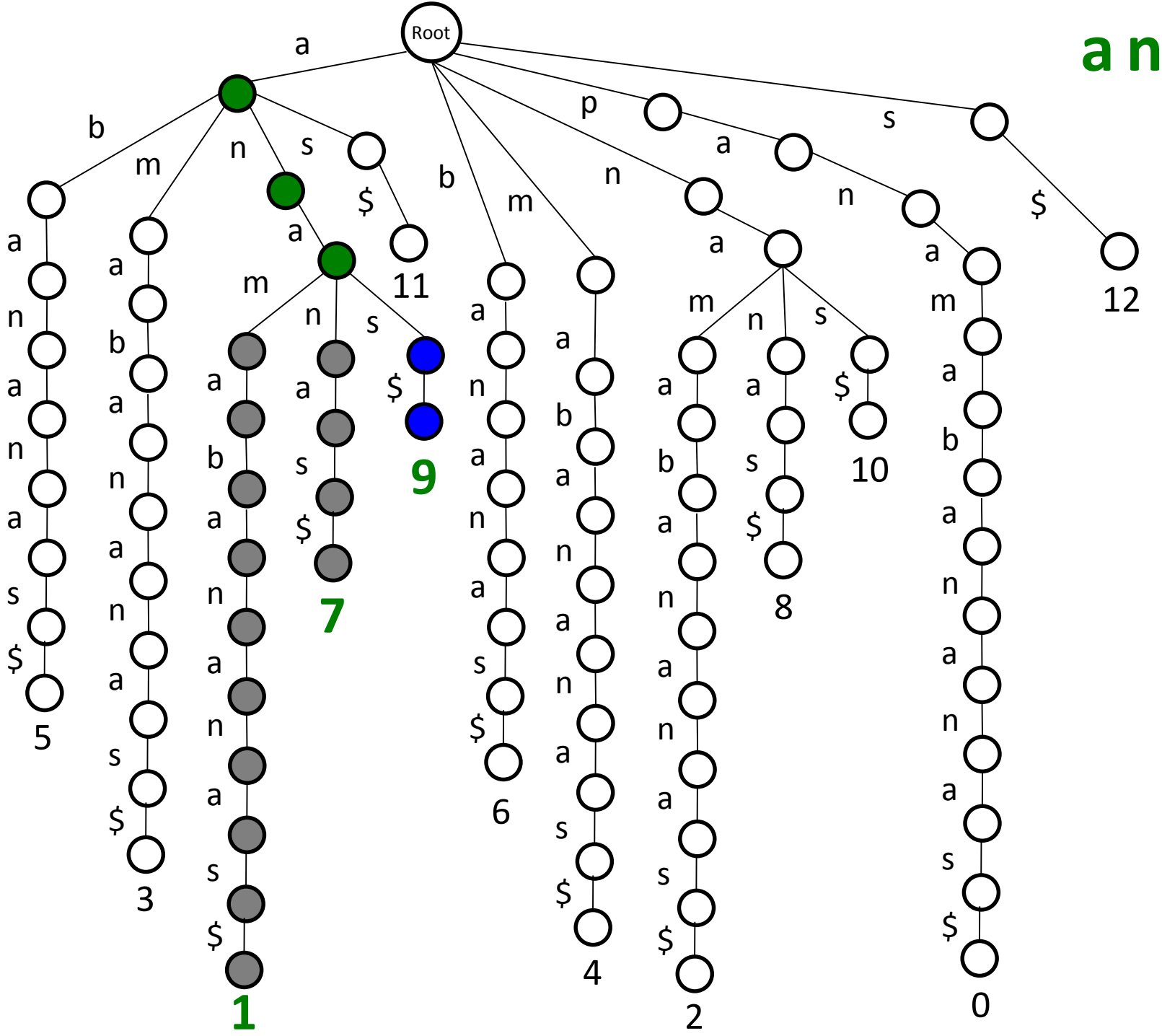
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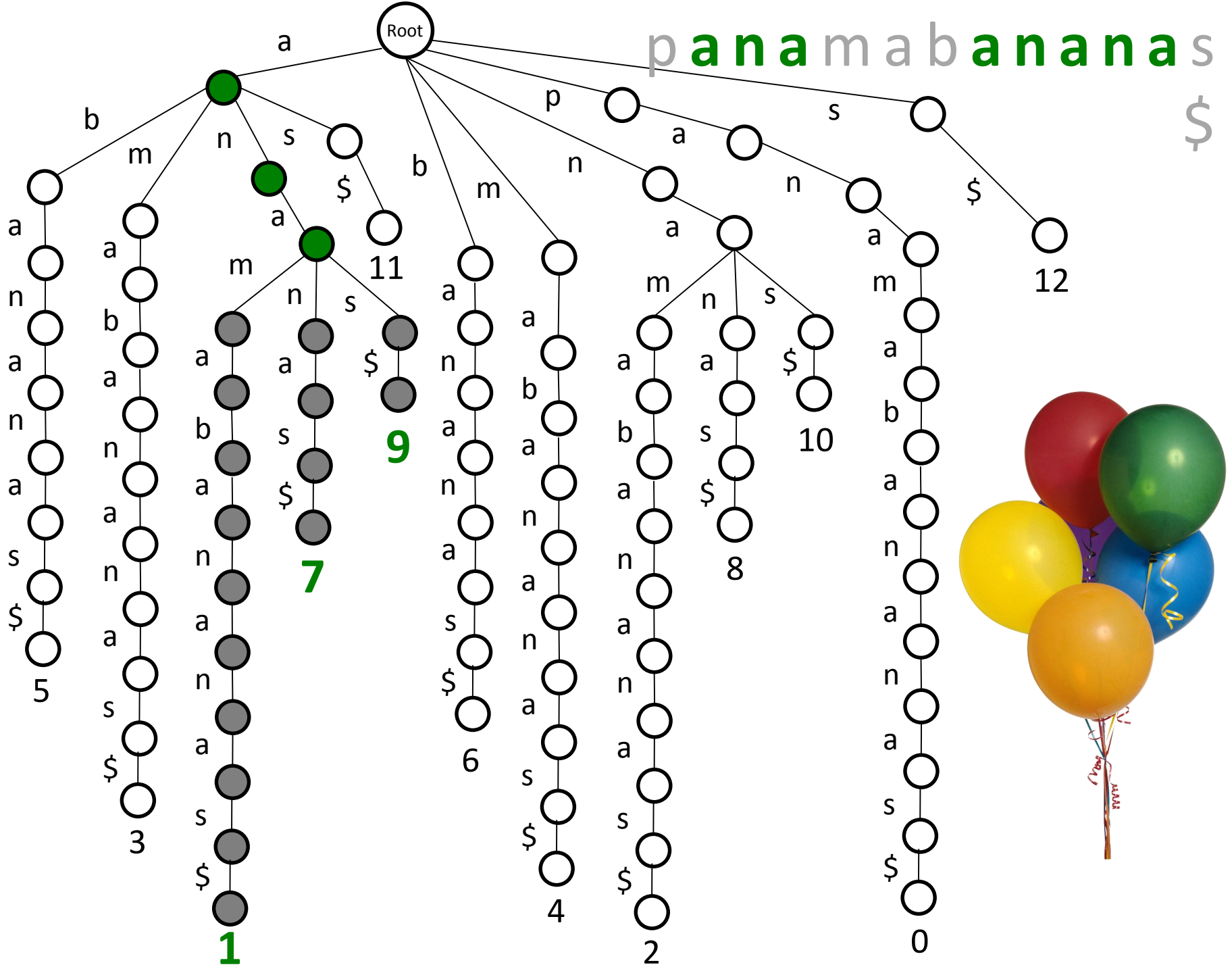
panamabanana$
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Memory Footprint of Suffix Trie

The suffix trie is formed from |*Text*| suffixes with total length:

$$|Text|*(|Text|-1)/2$$

For human genome:

- $|Text| \approx 3*10^9$

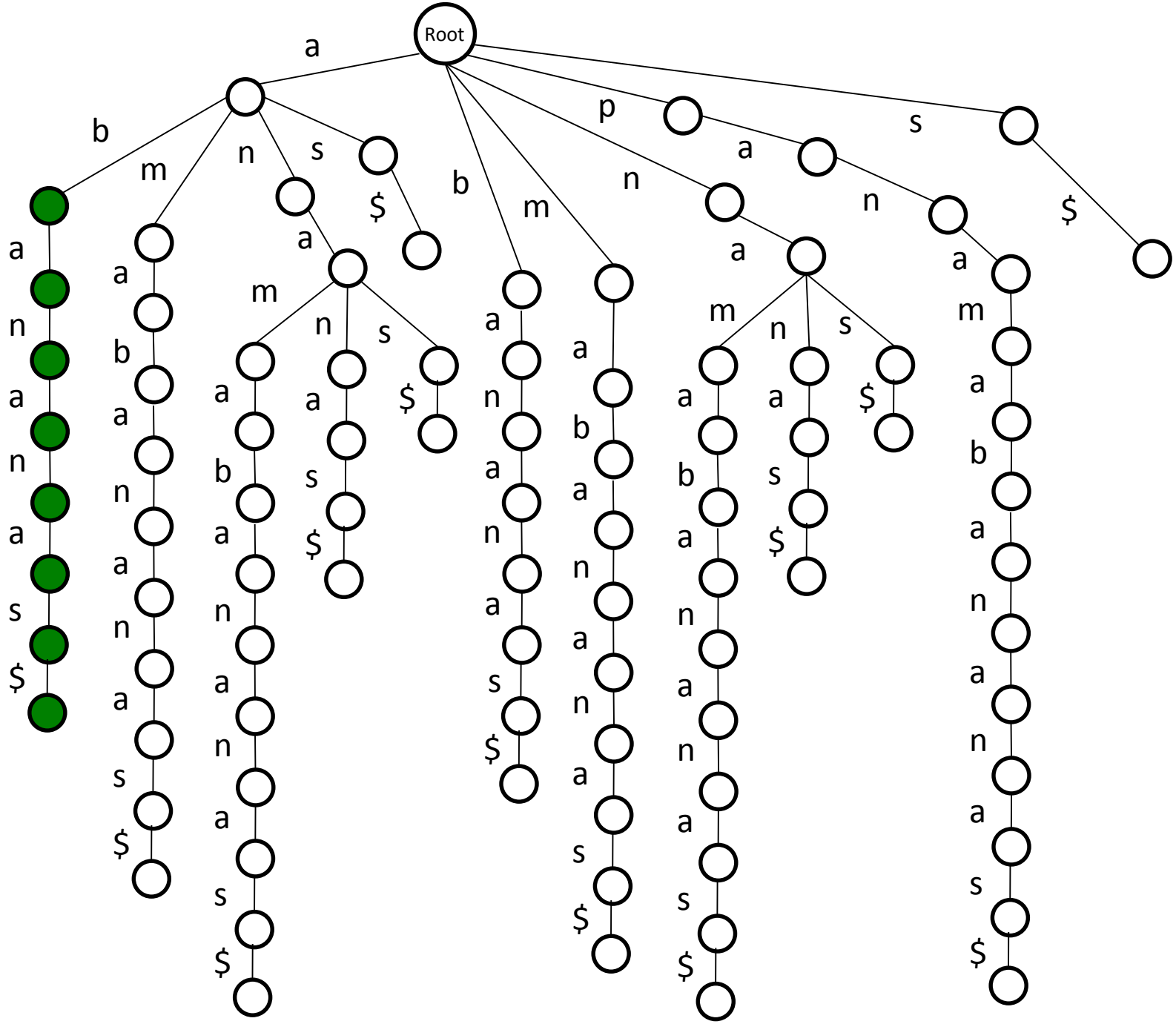
|*Text*| symbols

```
p a n a m a b a n a n a s $
  a n a m a b a n a n a s $
    n a m a b a n a n a s $
      a m a b a n a n a s $
        m a b a n a n a s $
          a b a n a n a s $
            b a n a n a s $
              a n a n a s $
                n a n a s $
                  a n a s $
                    n a s $
                      a s $
                        s $
                          $
```

|*Text*| suffixes

Outline

- From Genome Sequencing to Pattern Matching
- Brute Force Approach to Pattern Matching
- Herding Patterns into Trie
- Herding Text into Suffix Trie
- **From Suffix Tries to Suffix Trees**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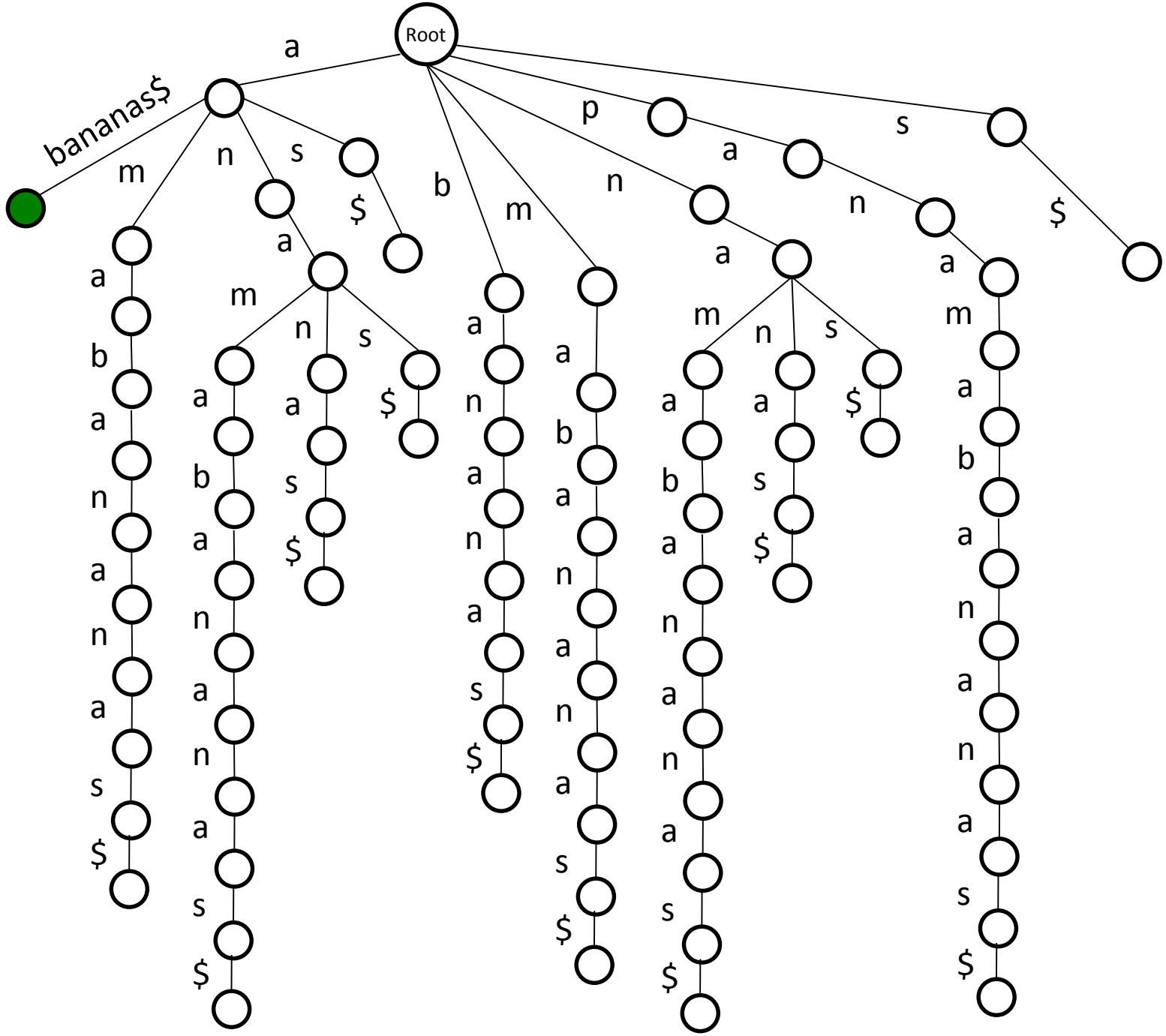
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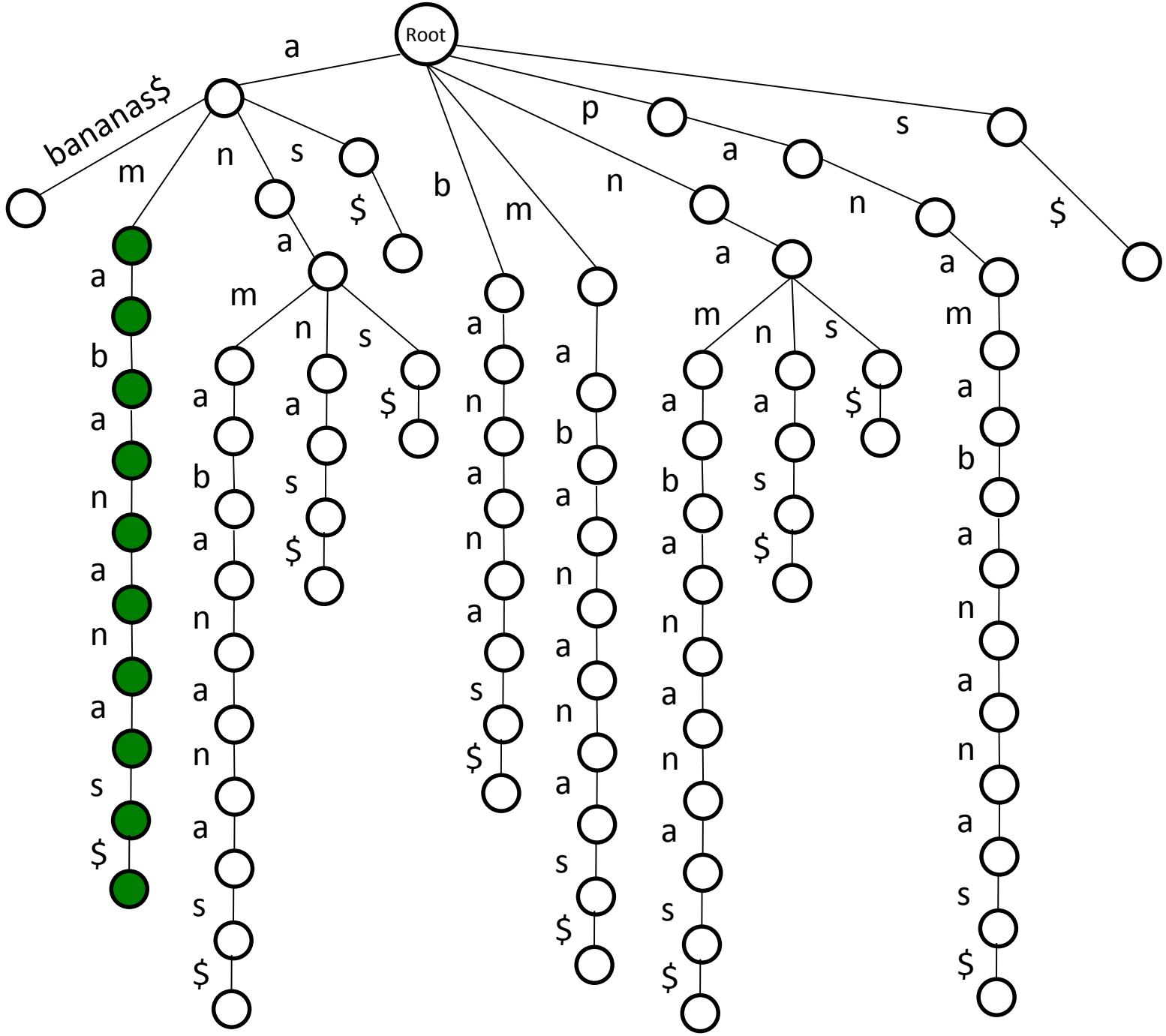
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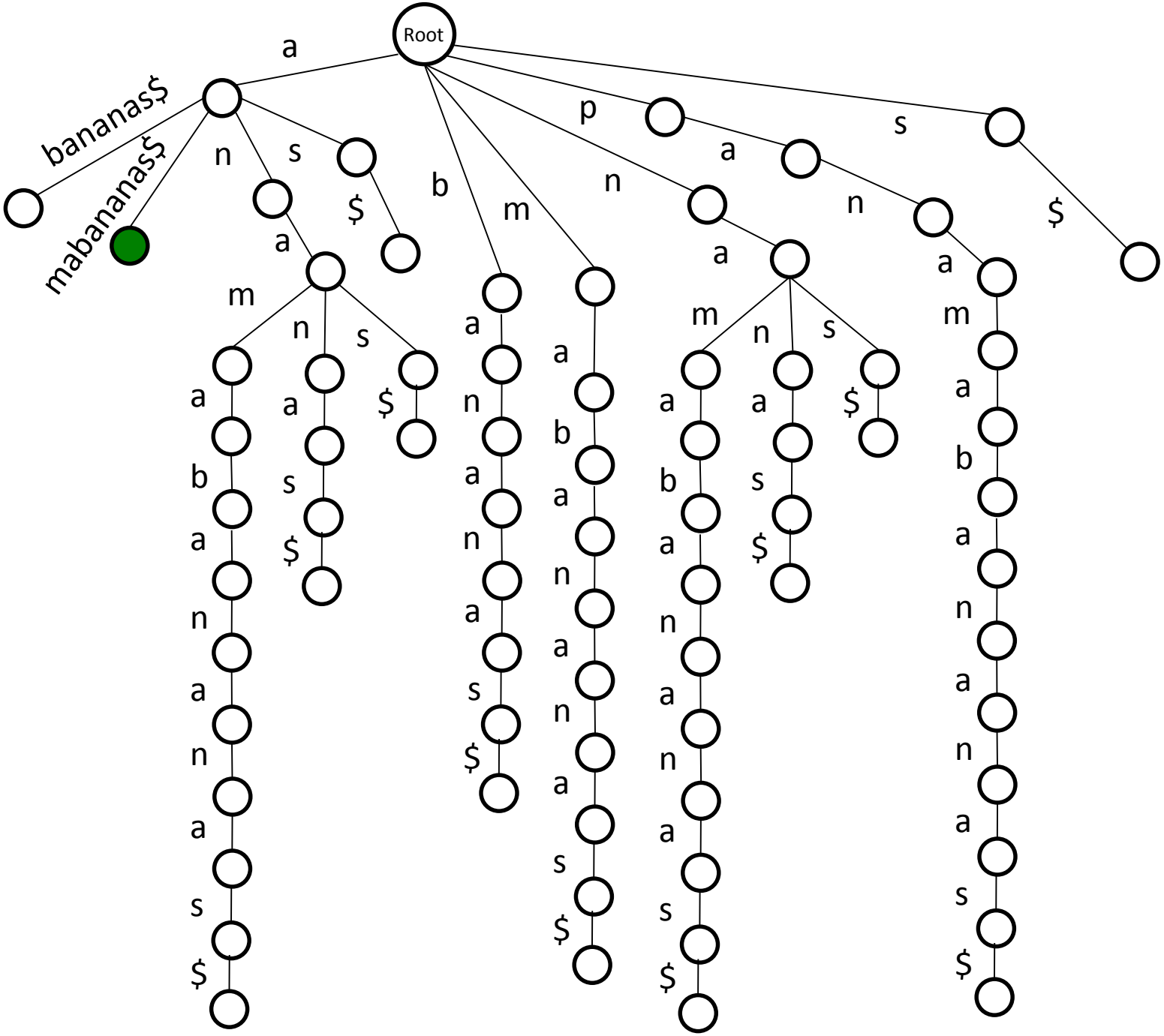
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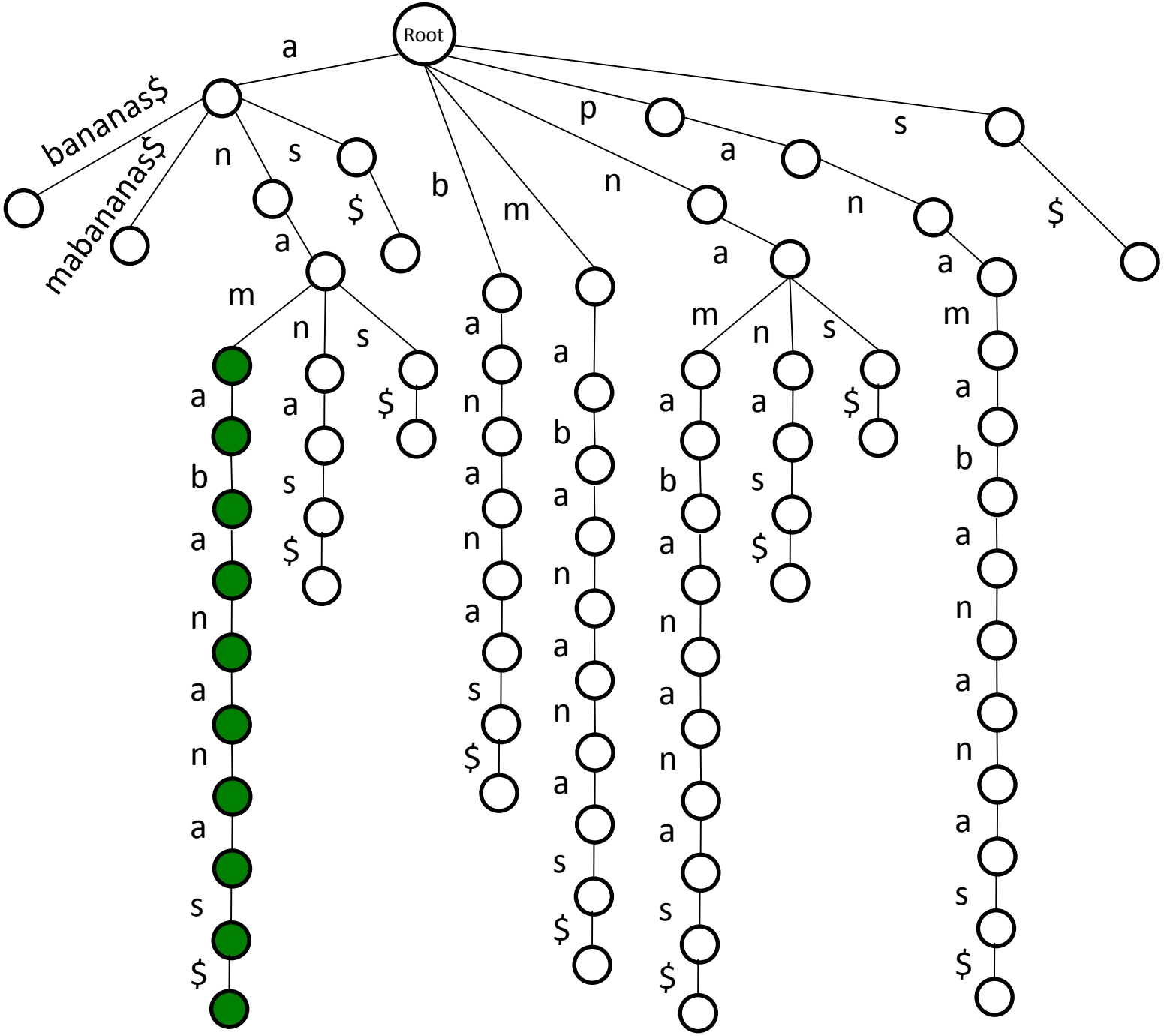
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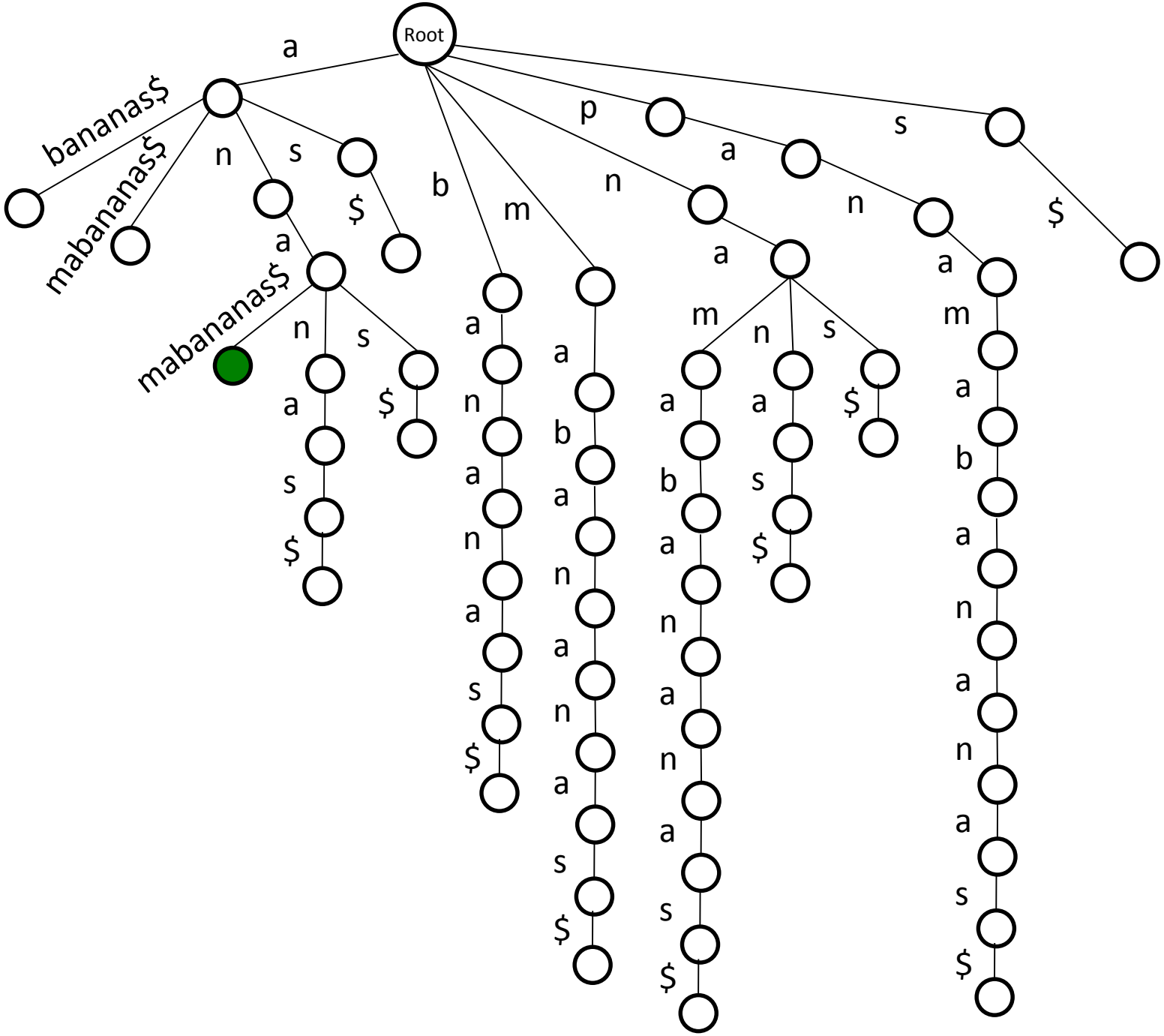
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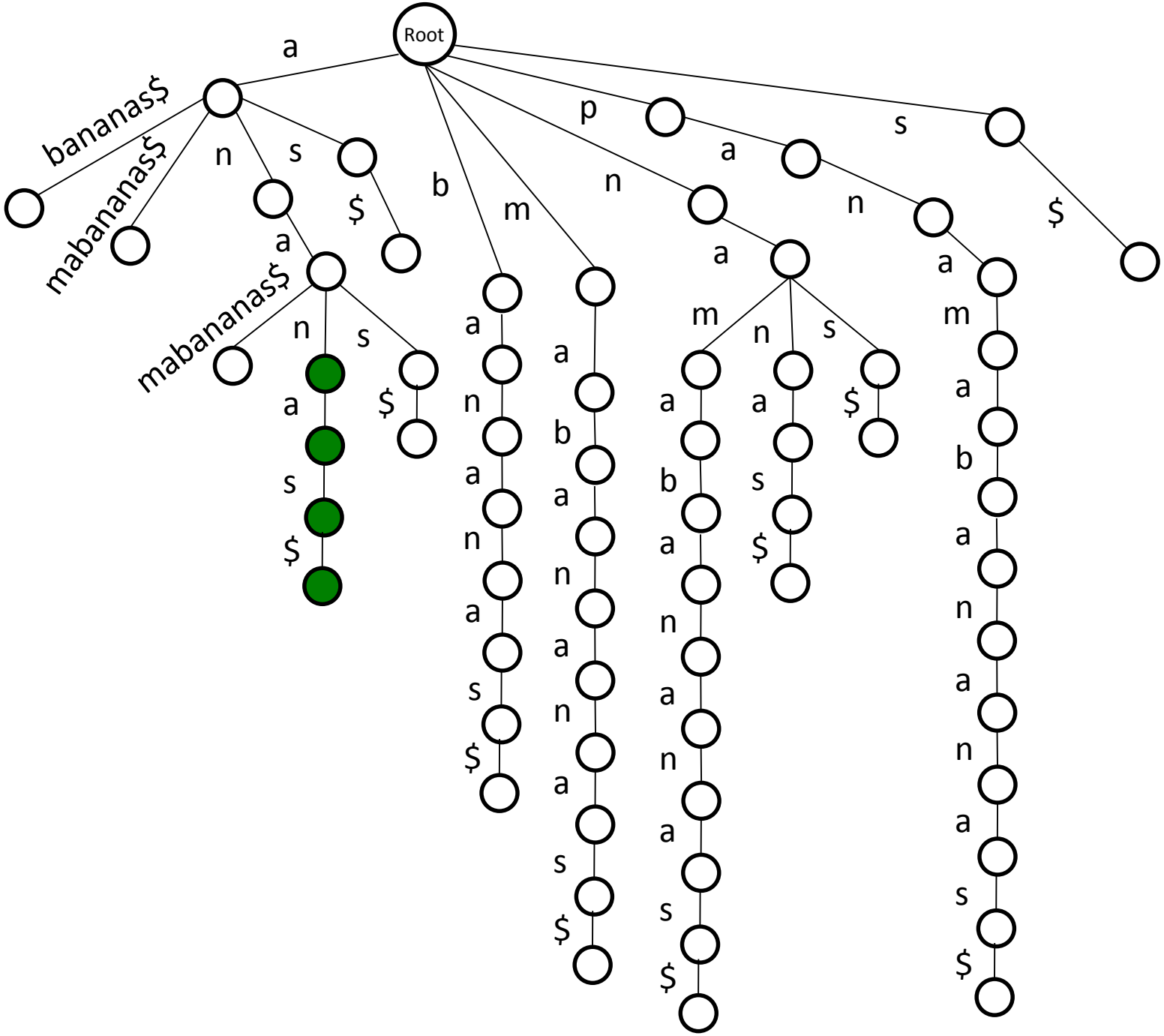
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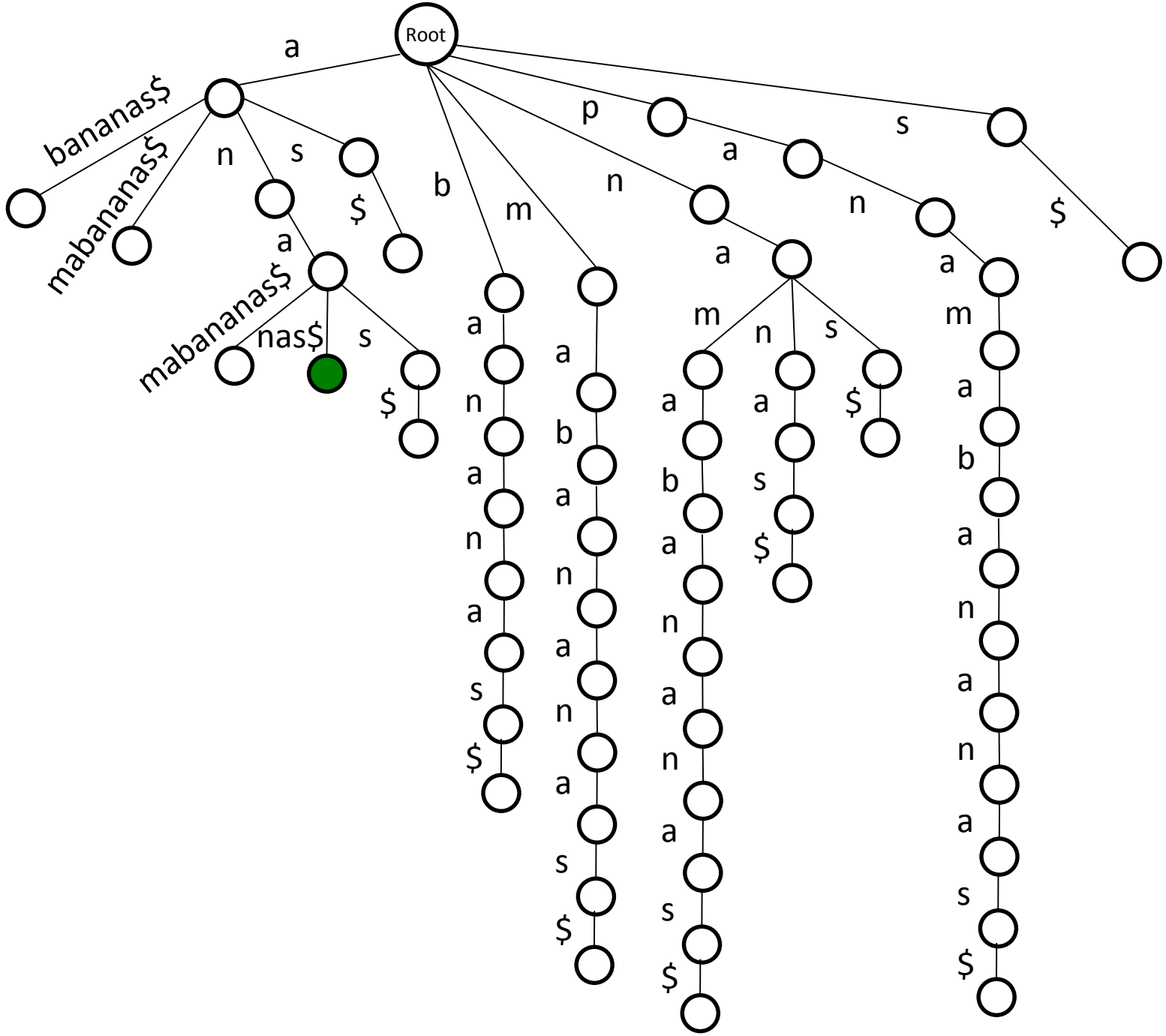
Root
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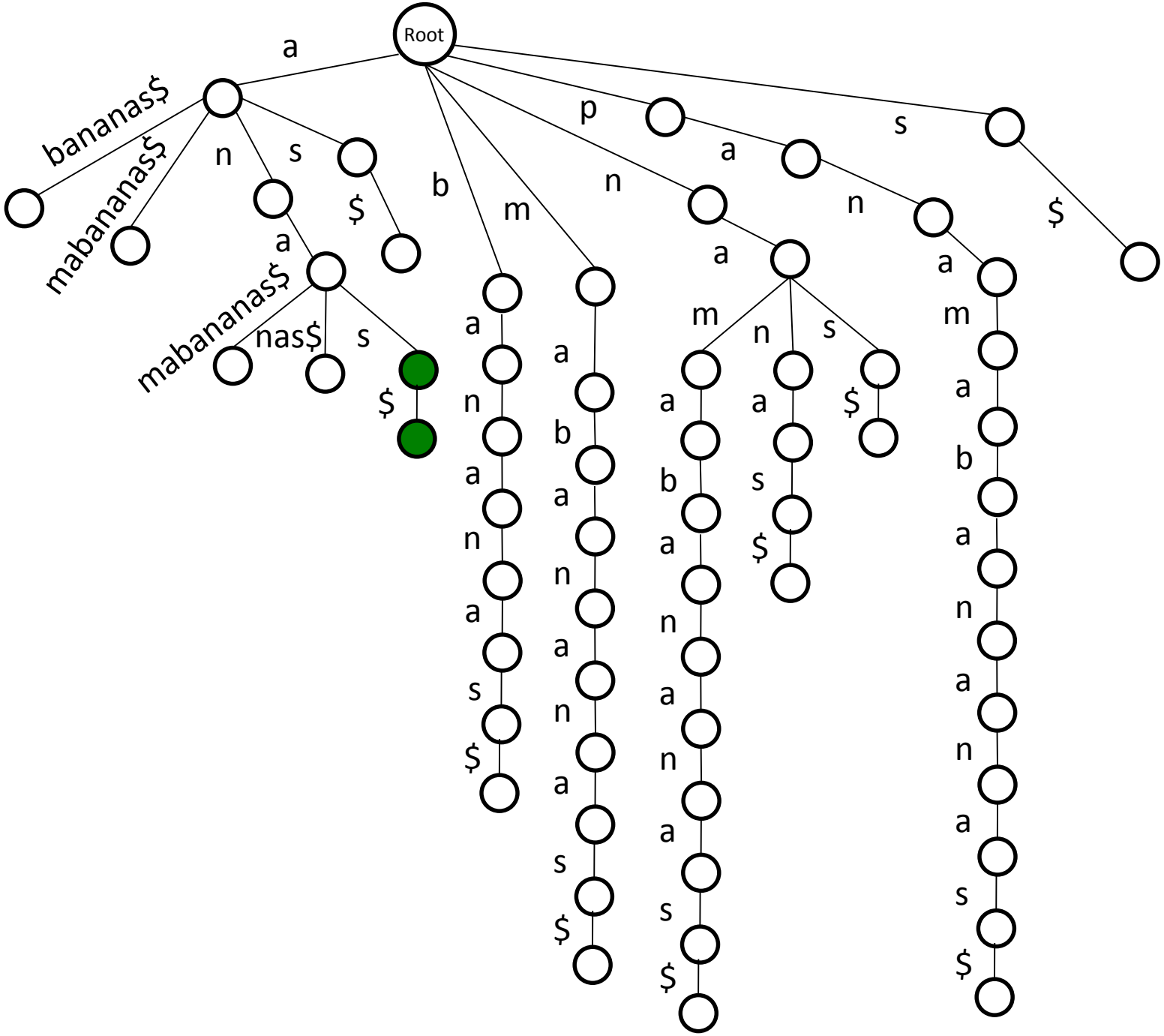
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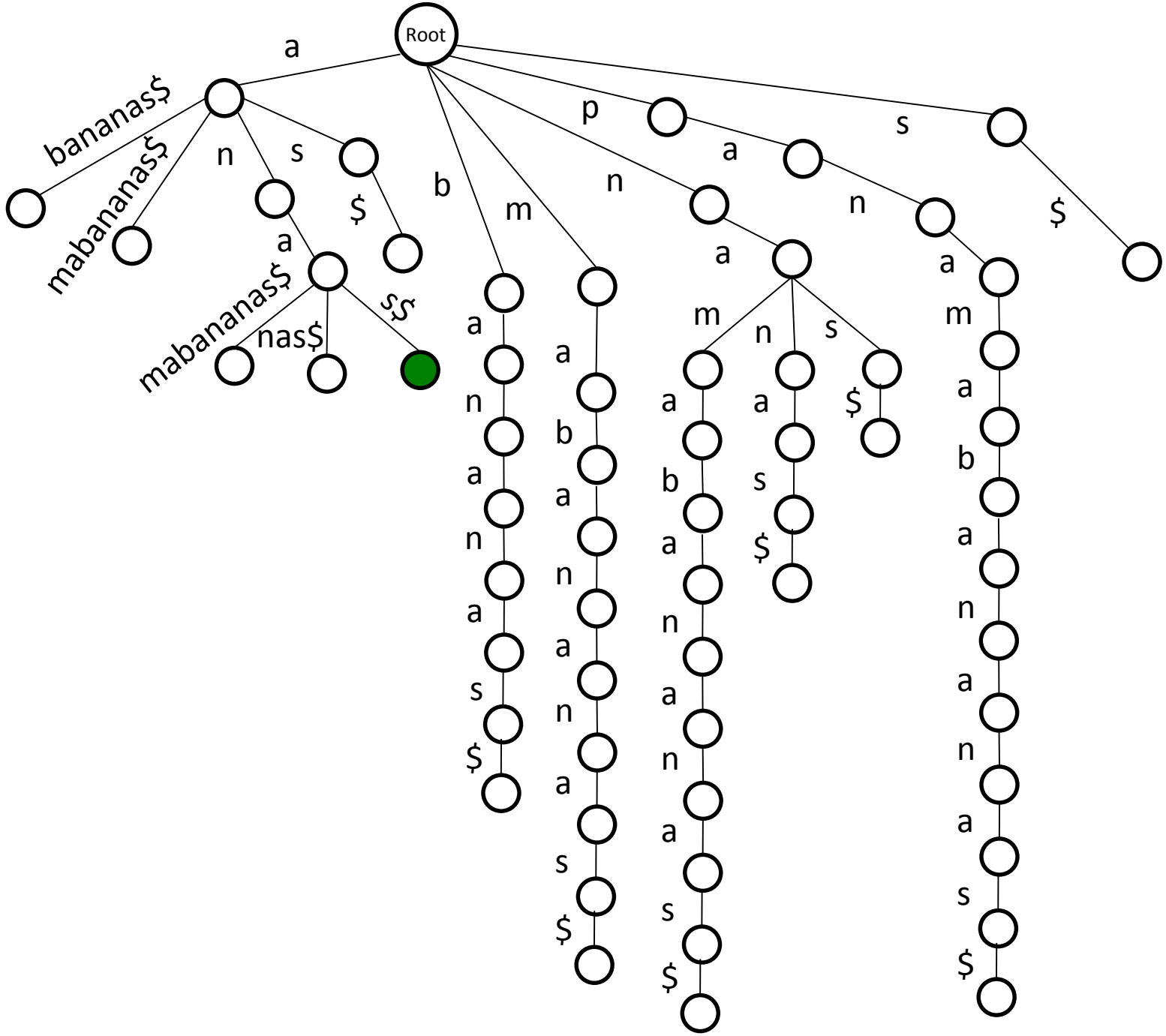
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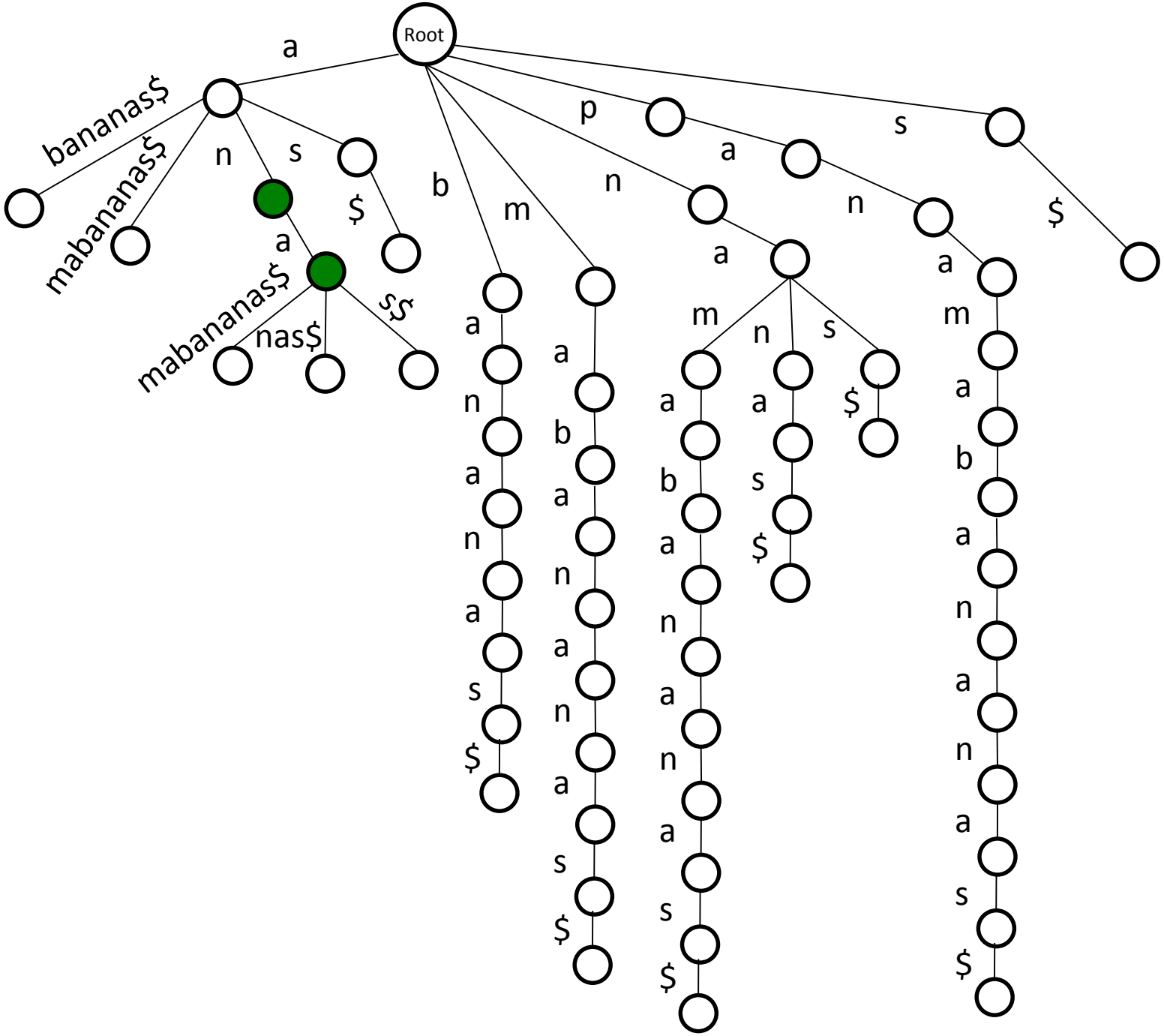
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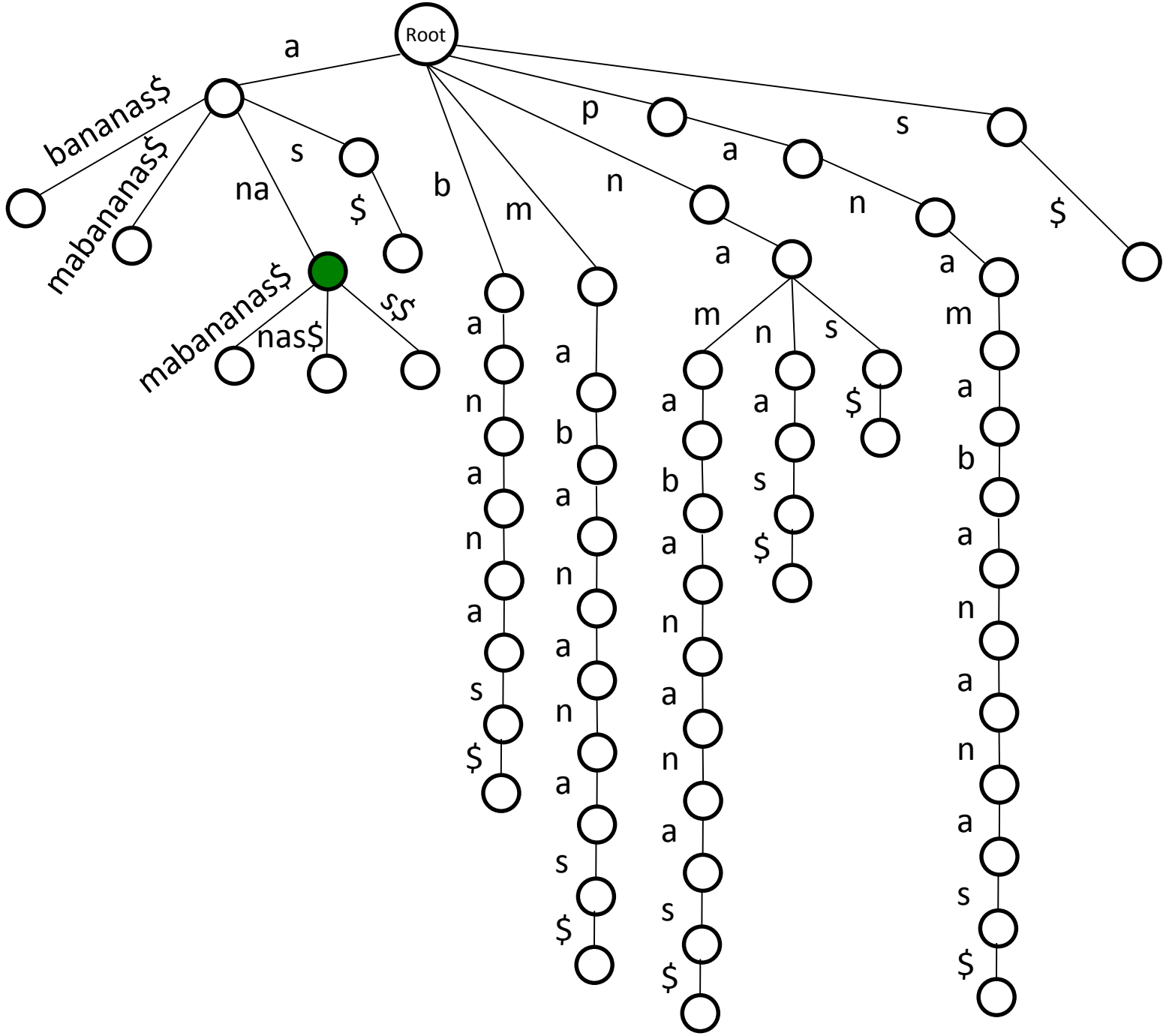
Root
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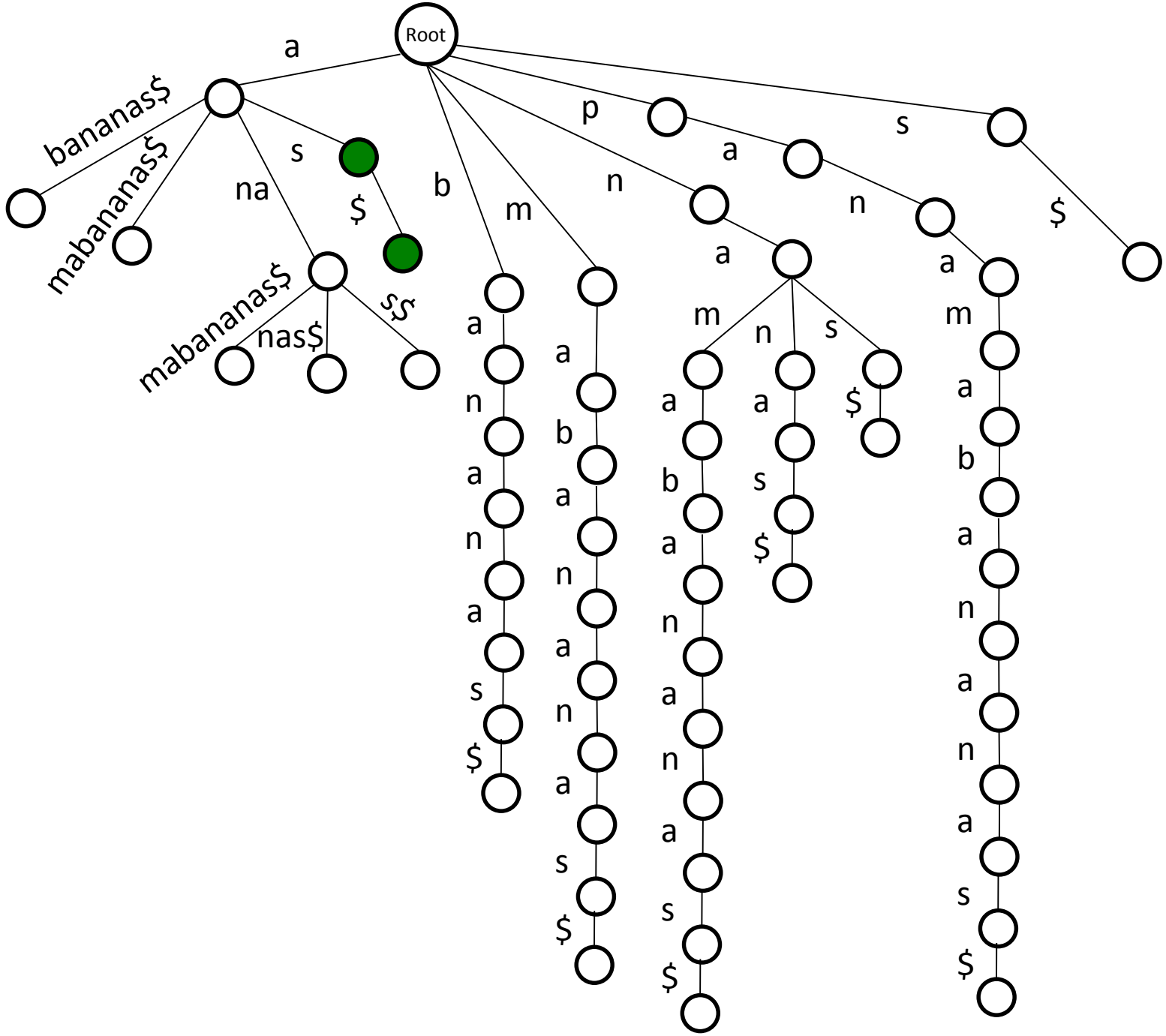
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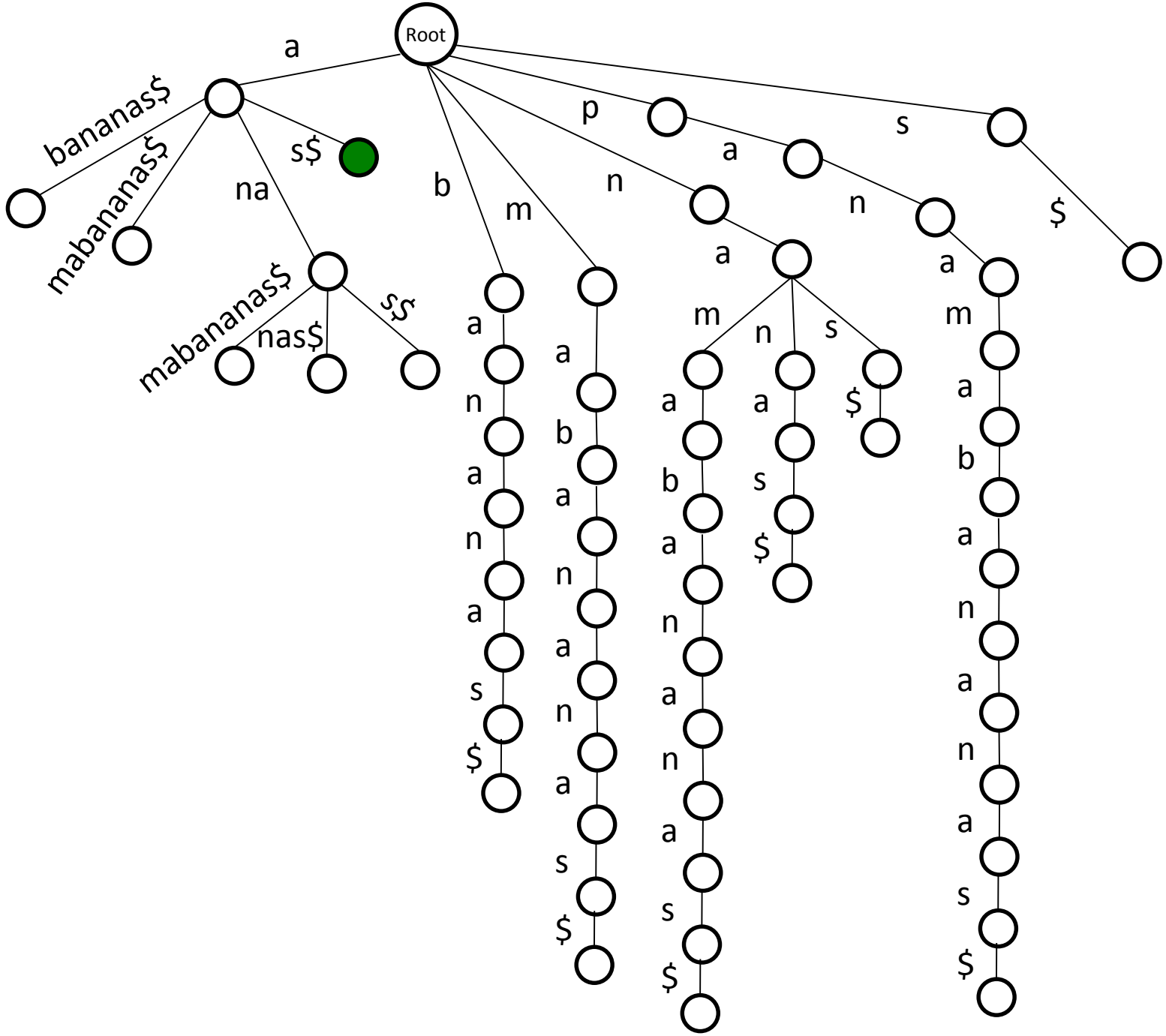
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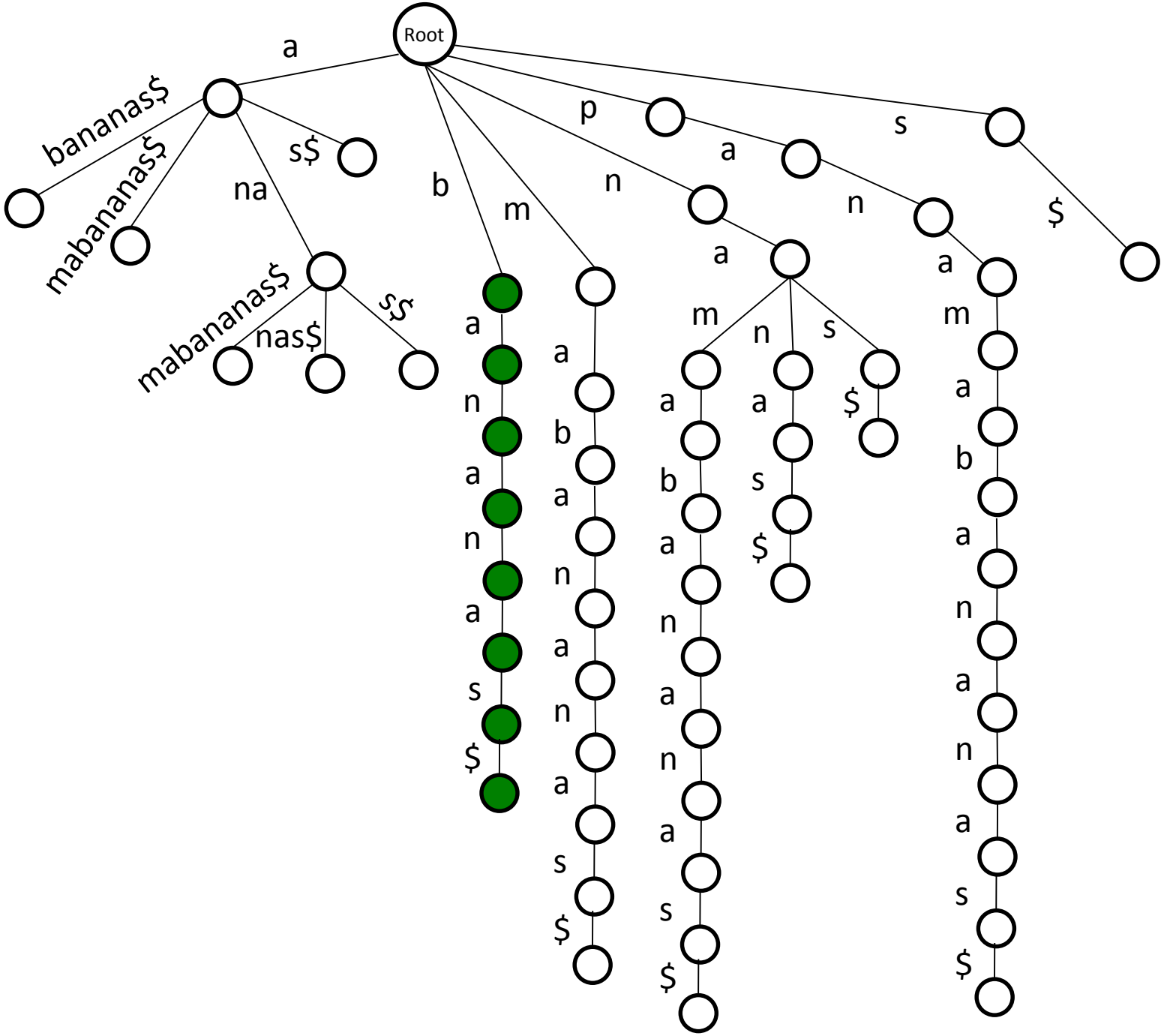
Root
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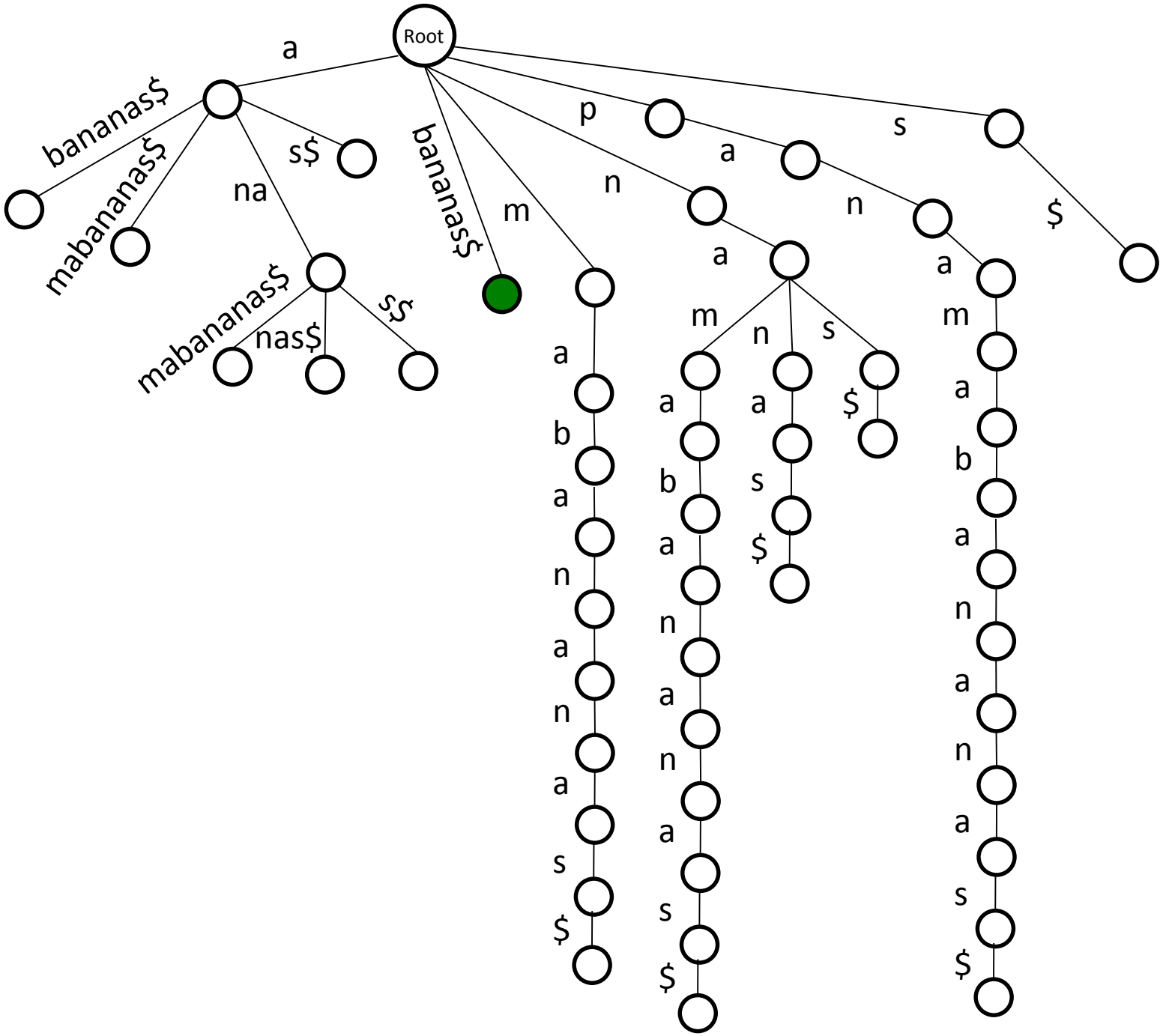
Root
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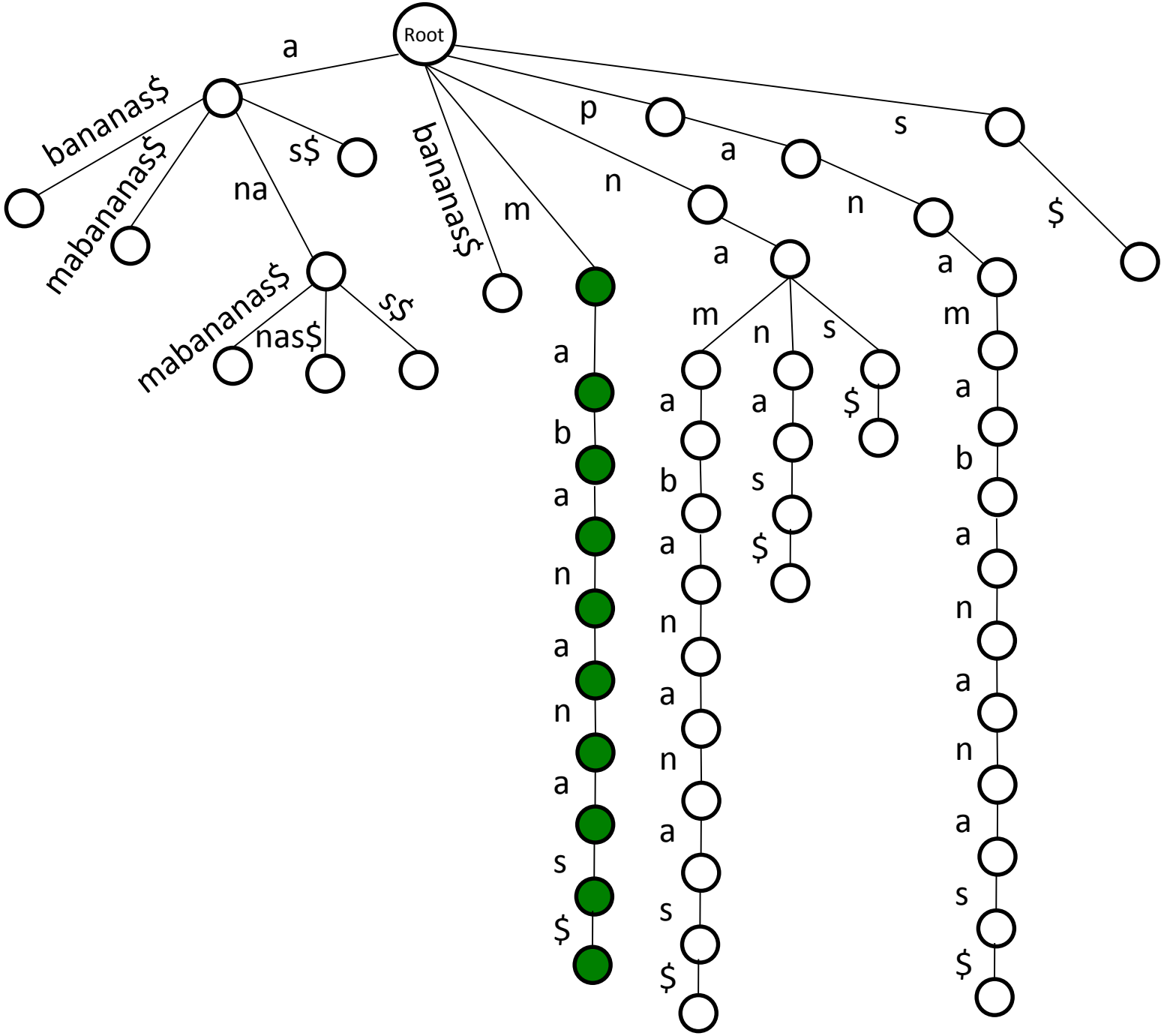
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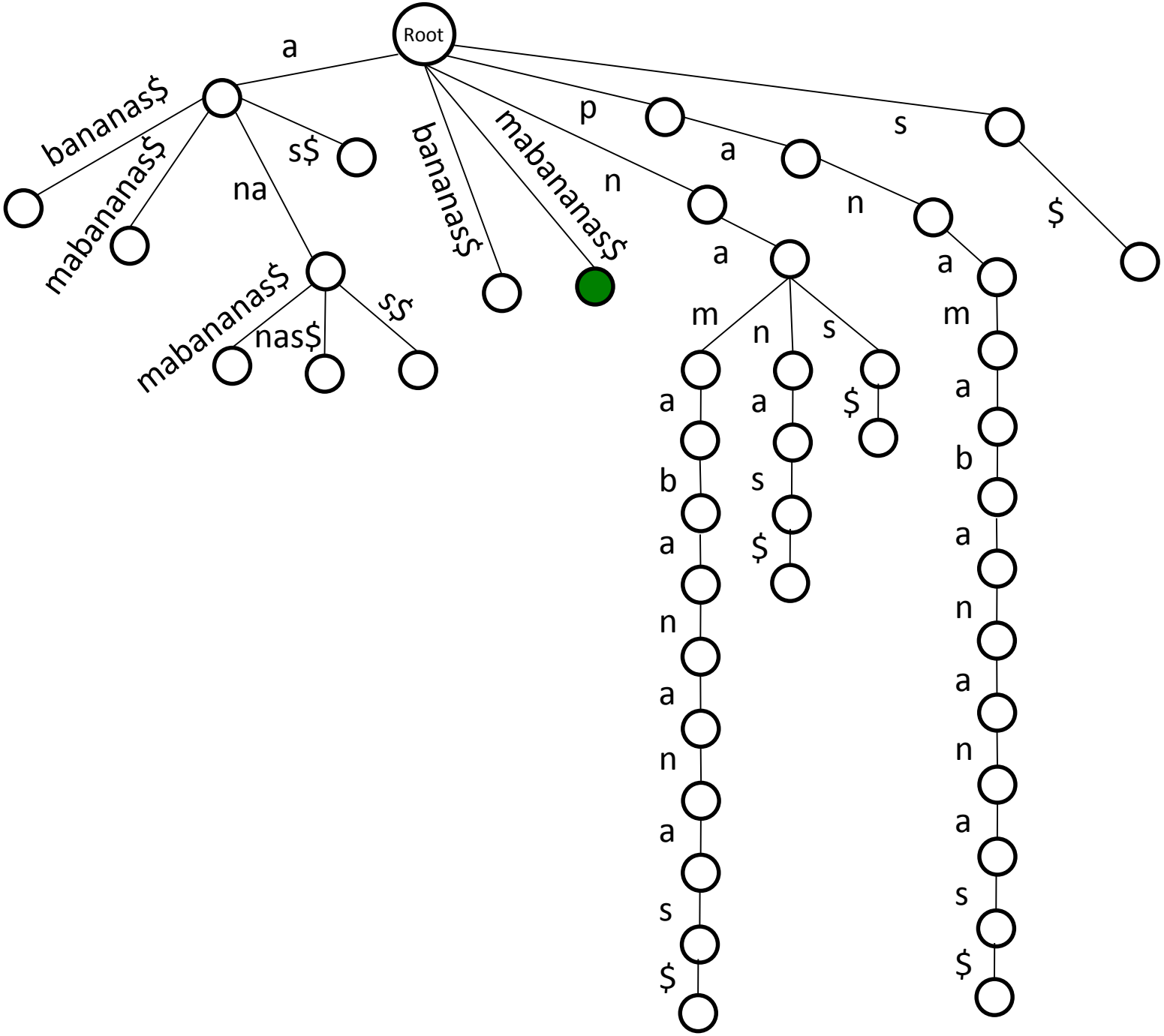
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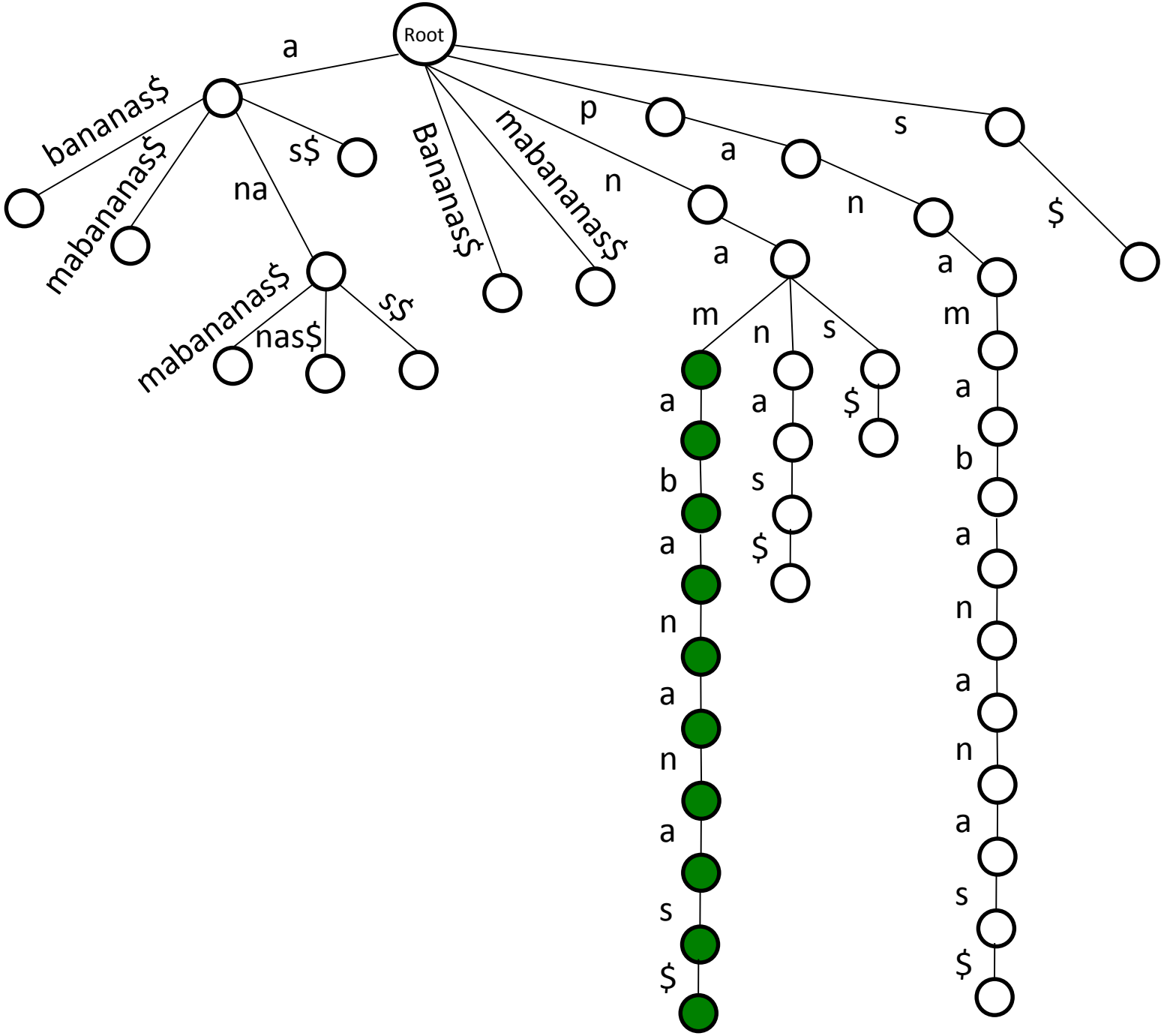
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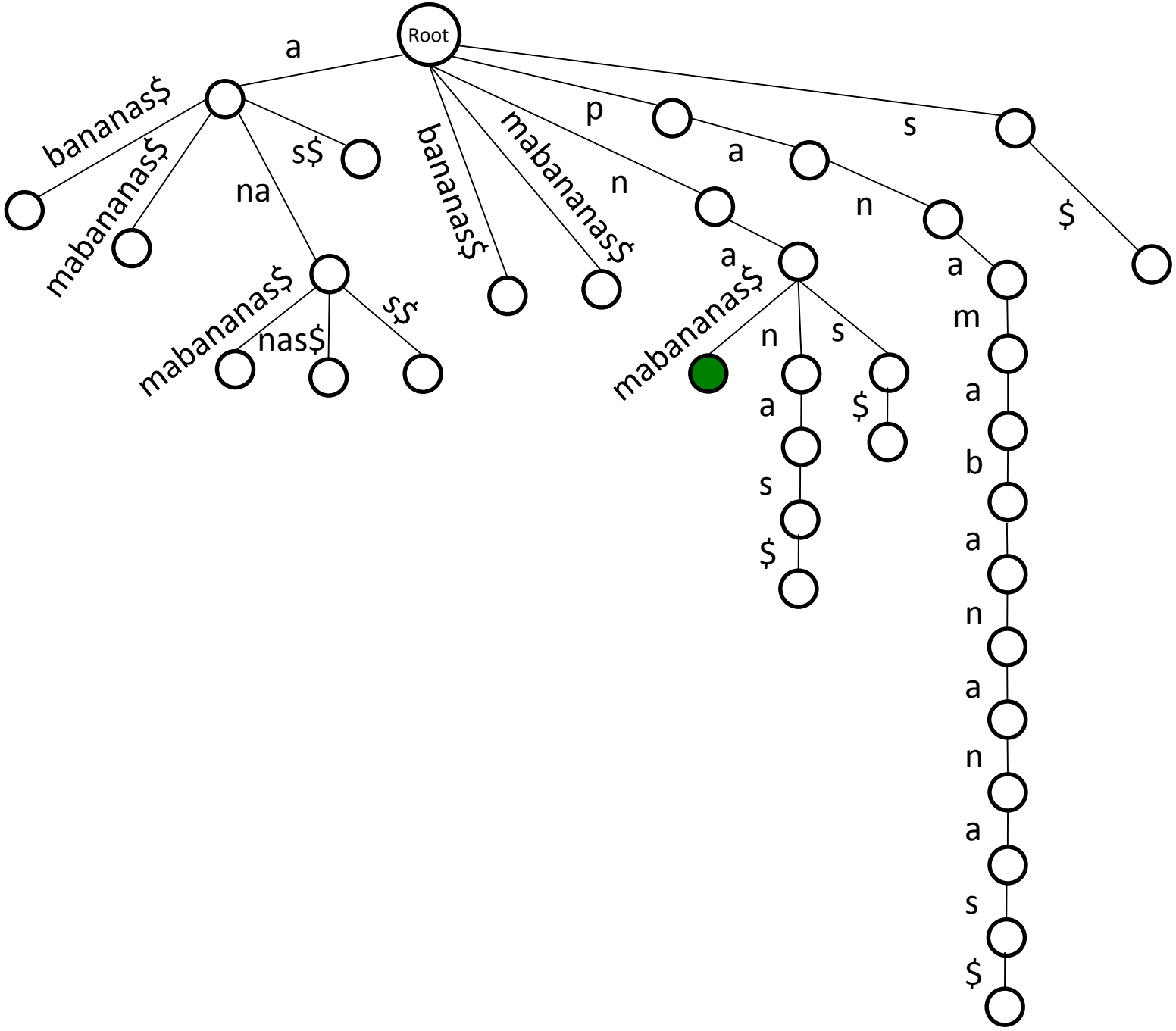
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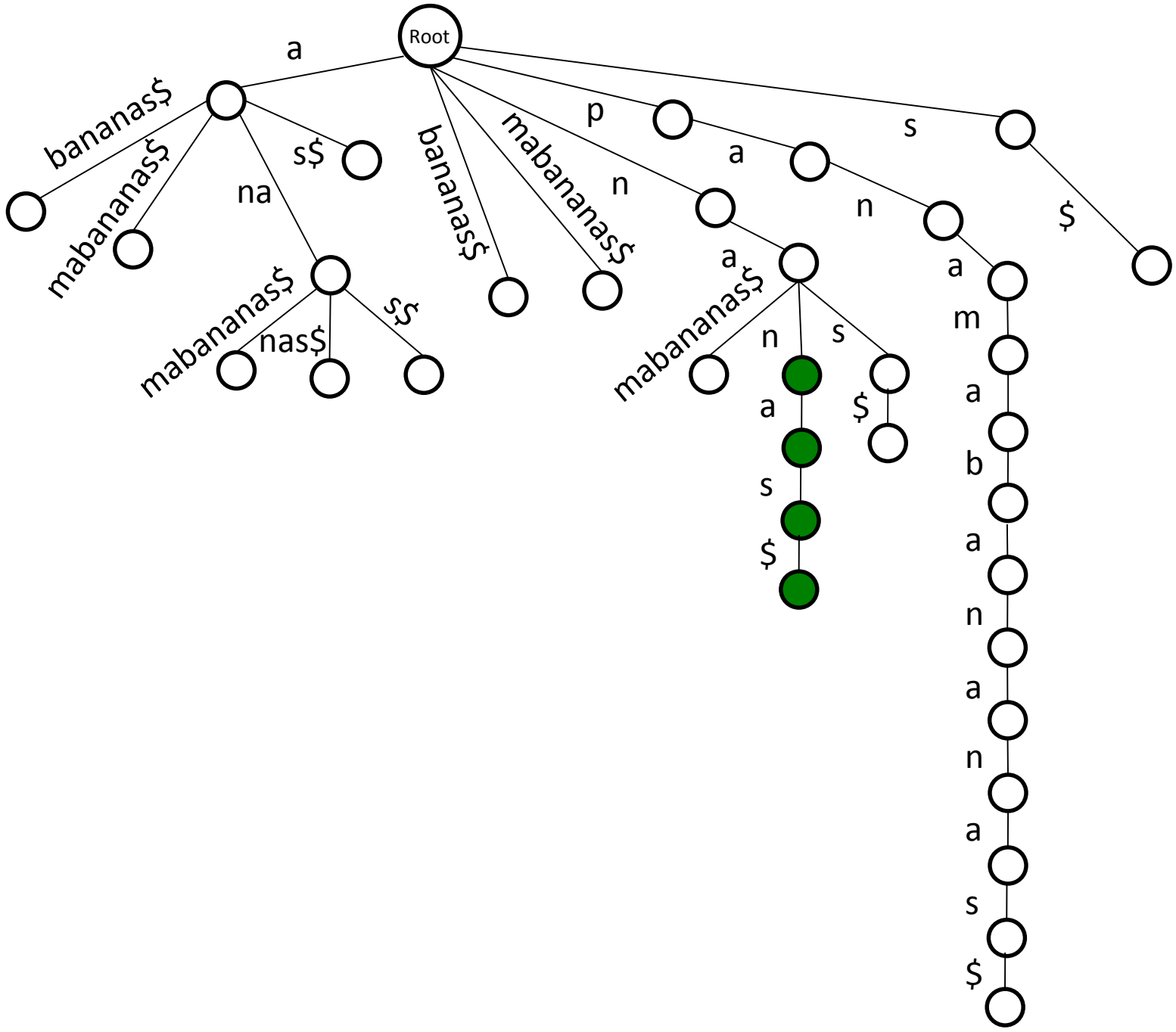
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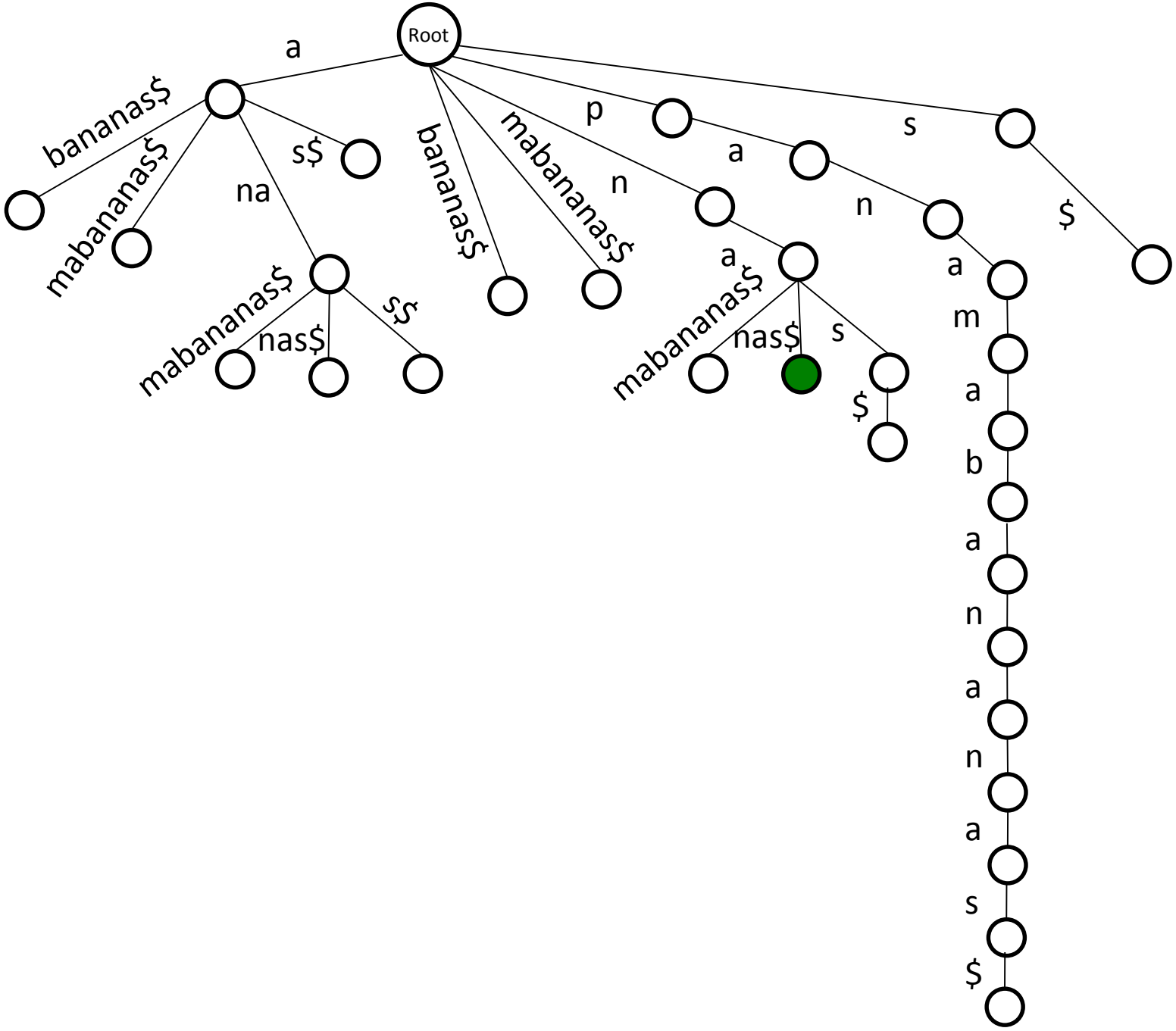
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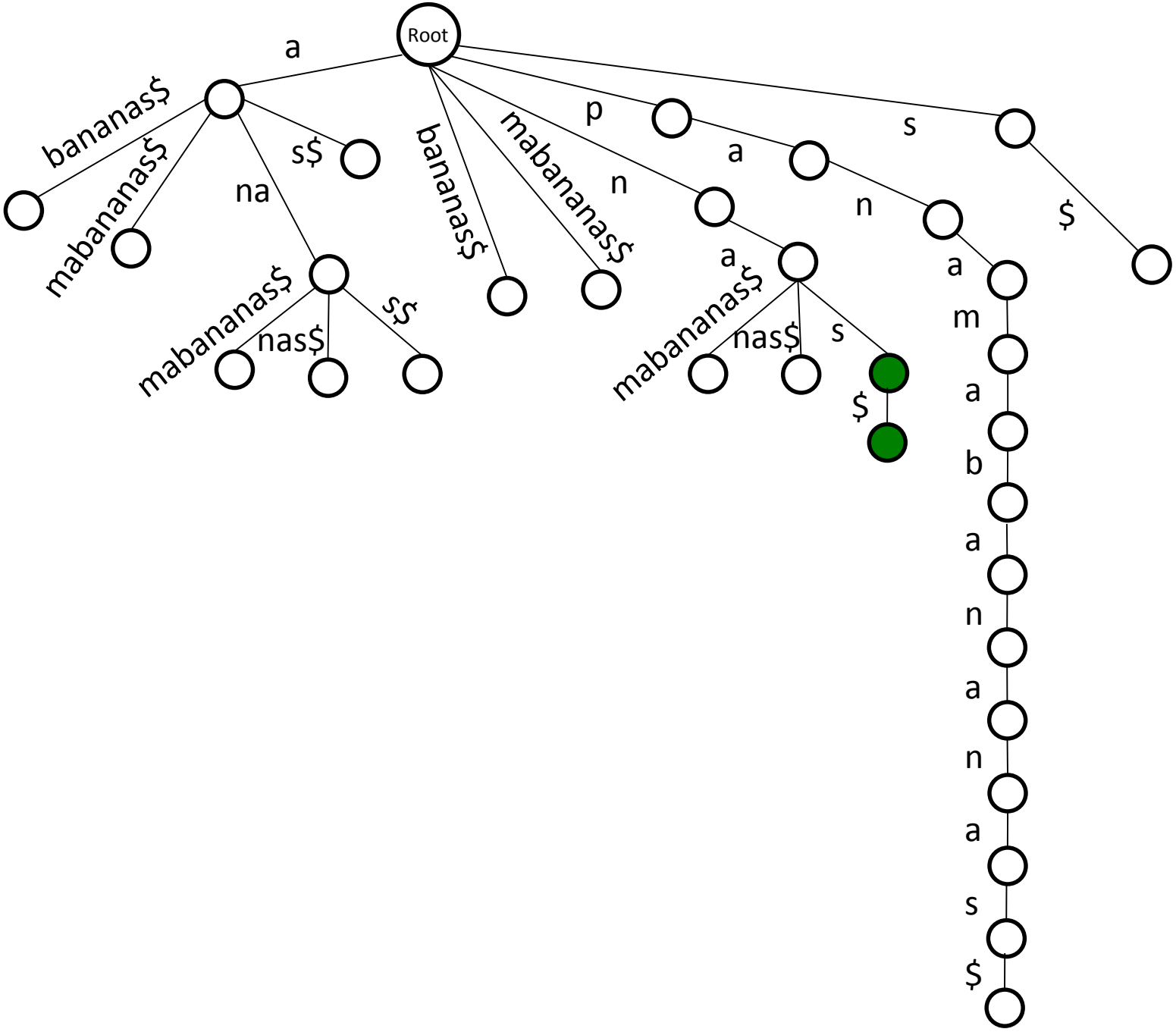
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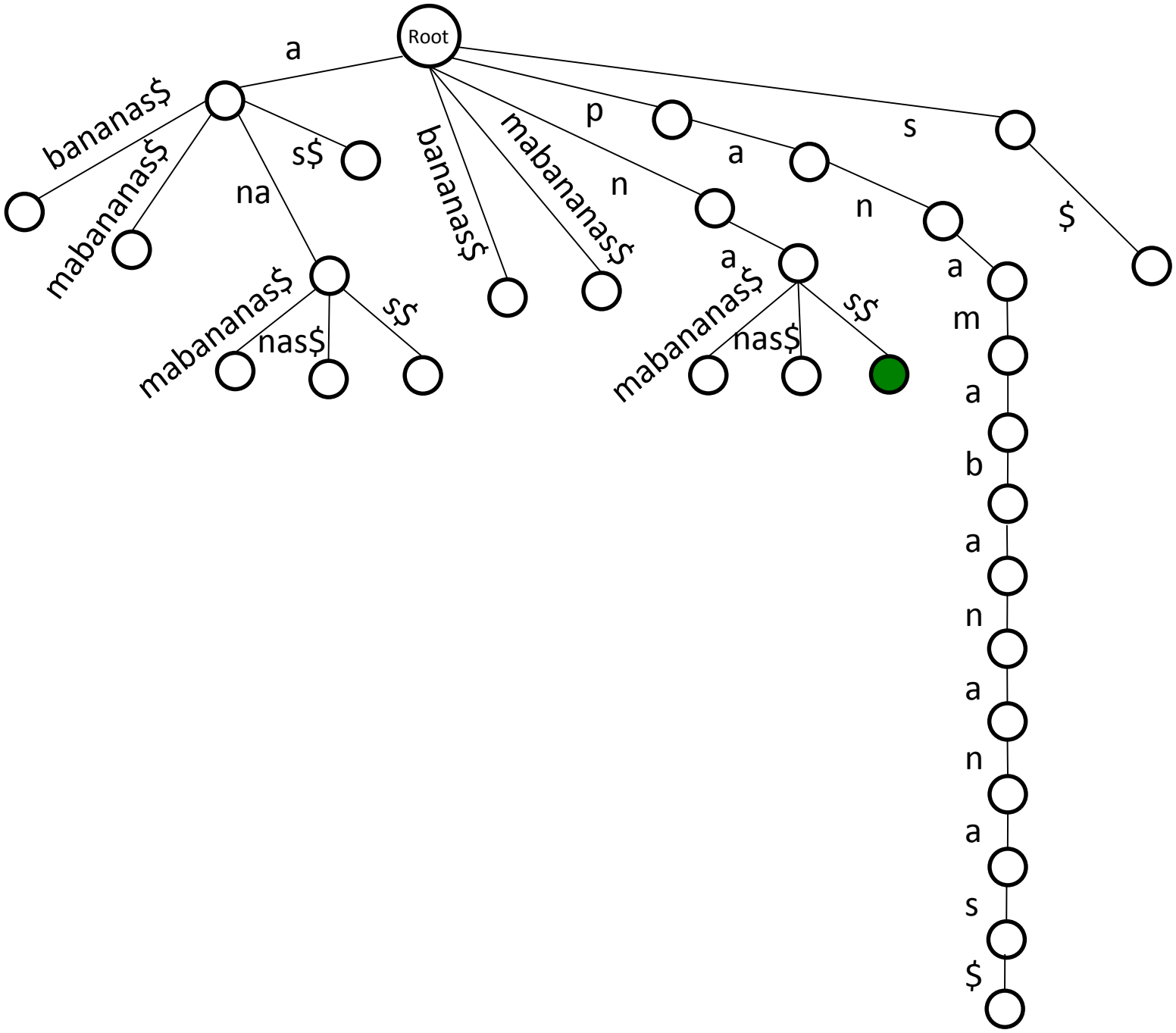
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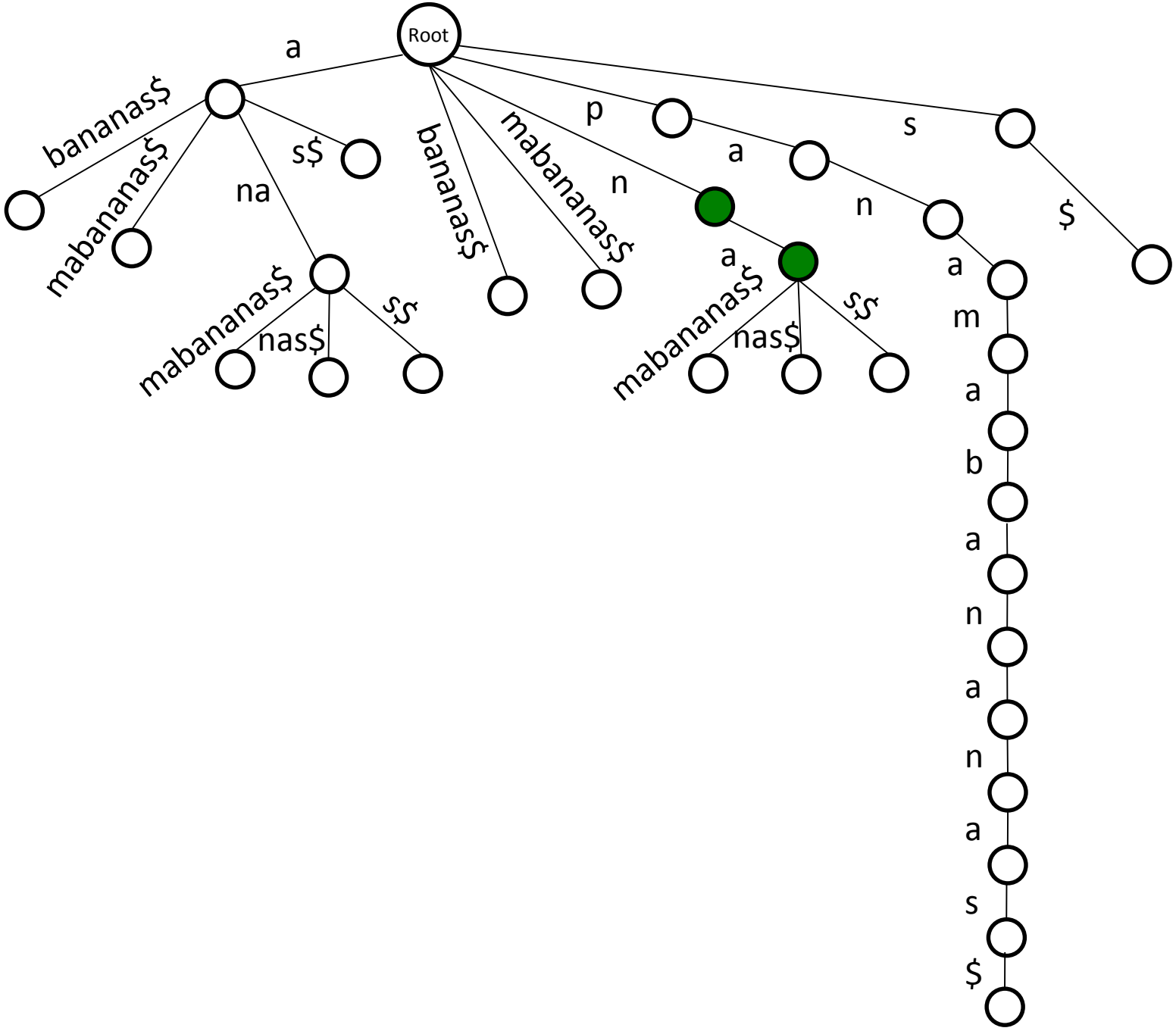
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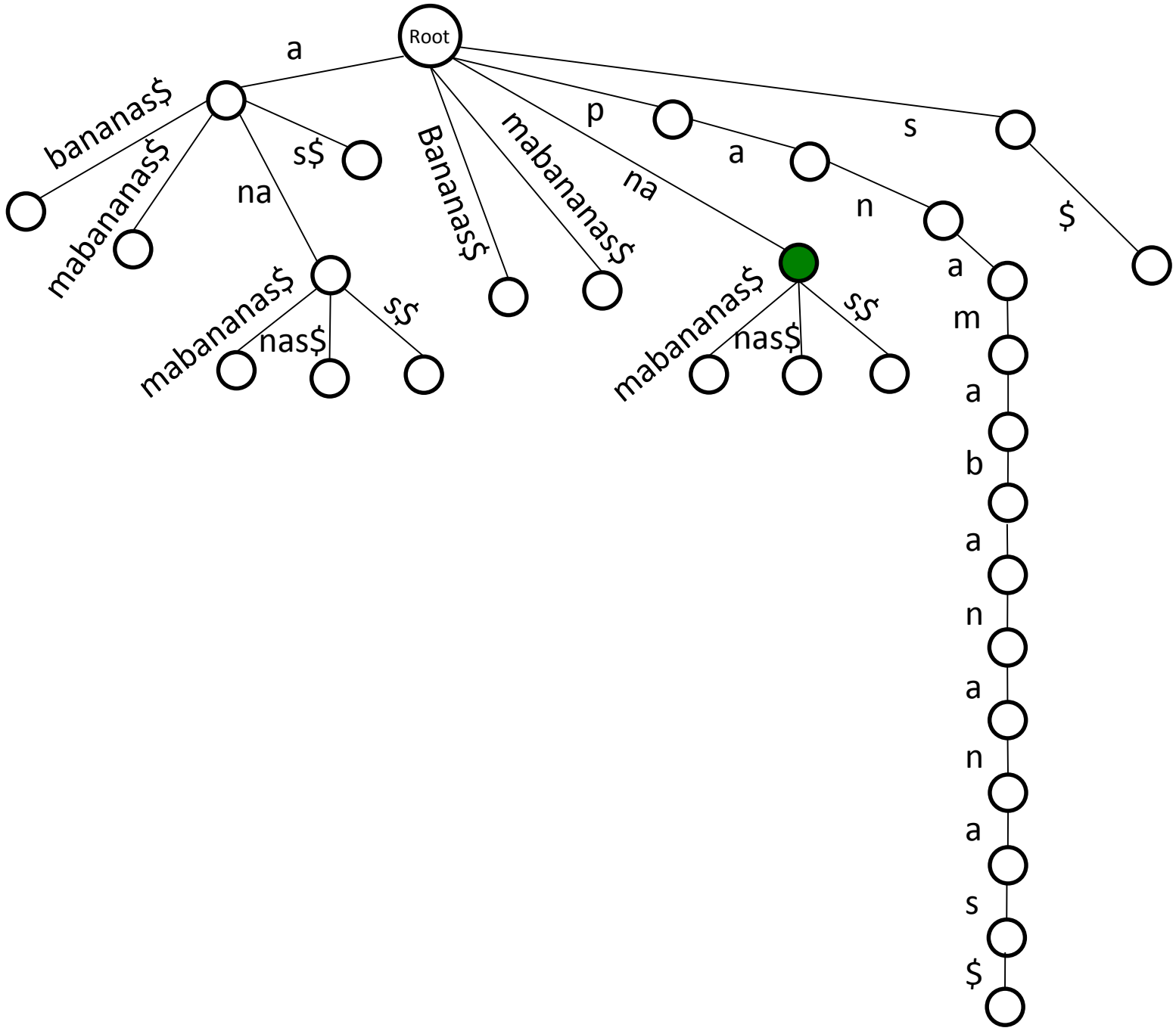
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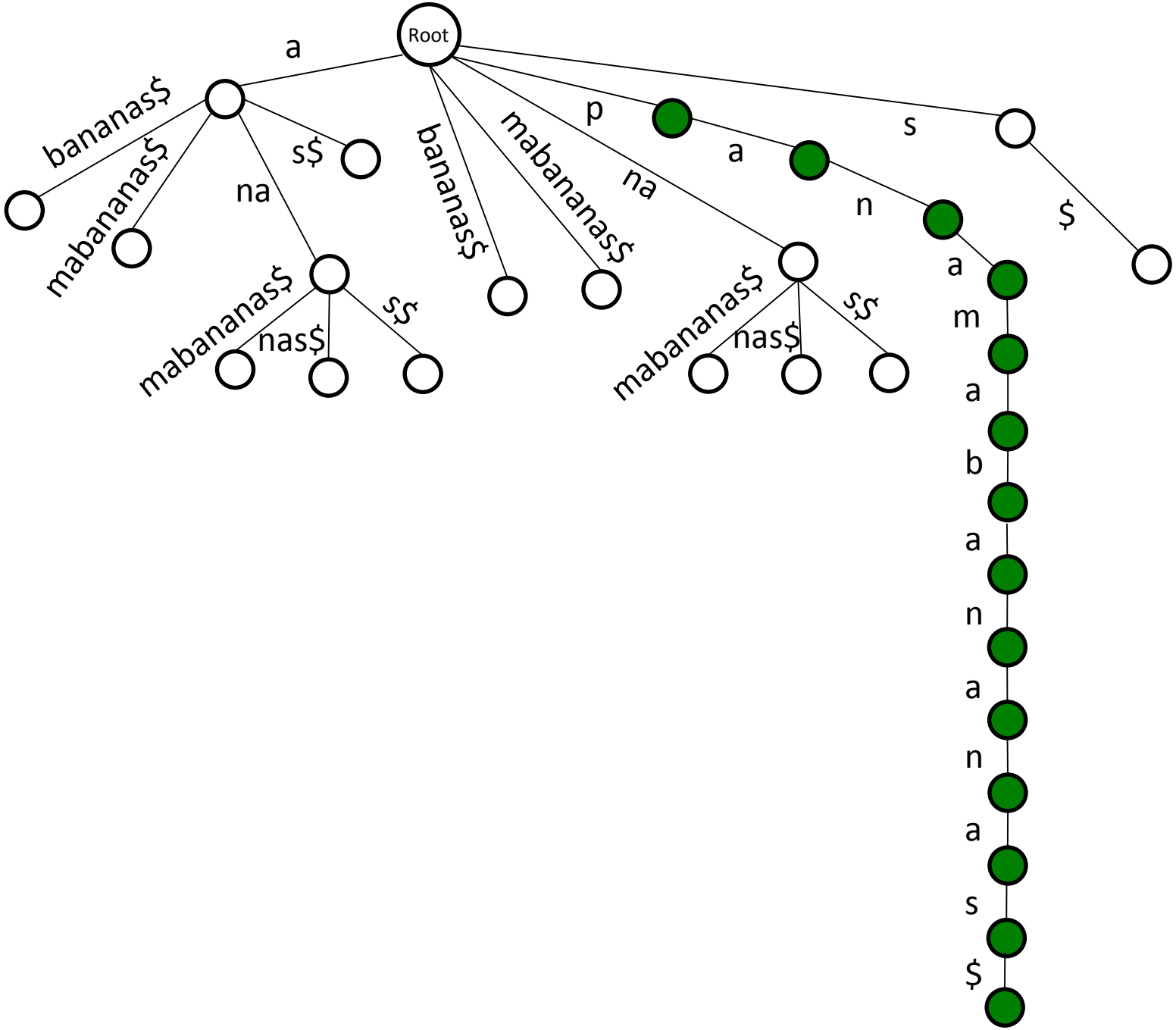
Root
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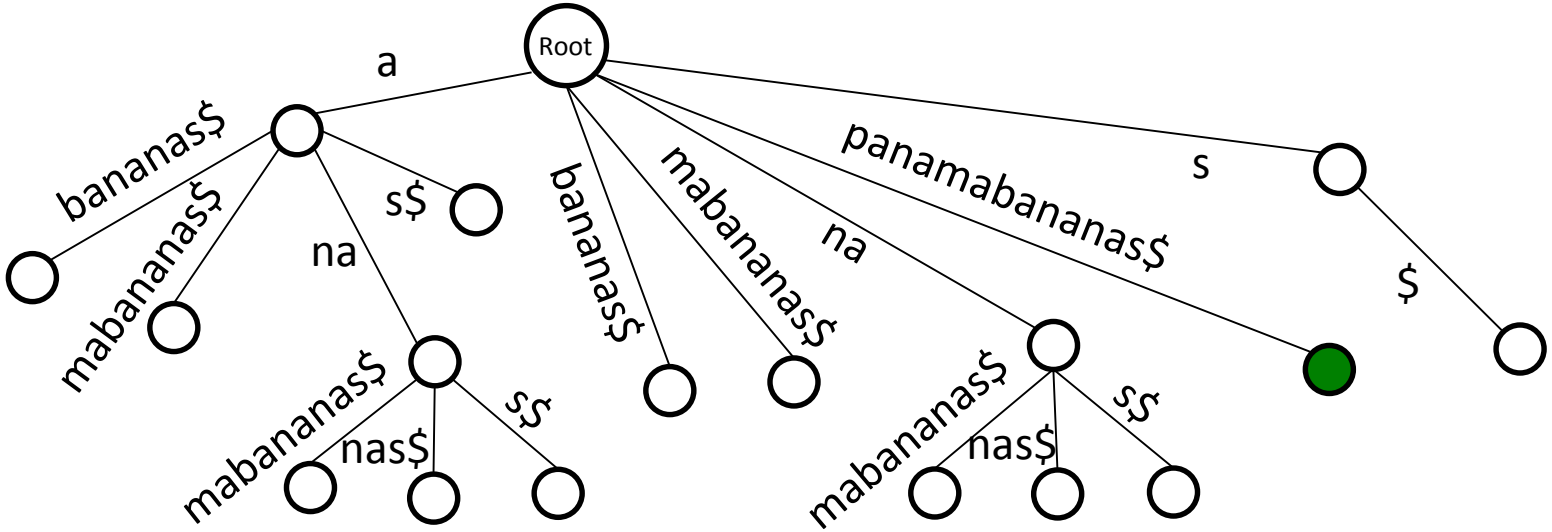
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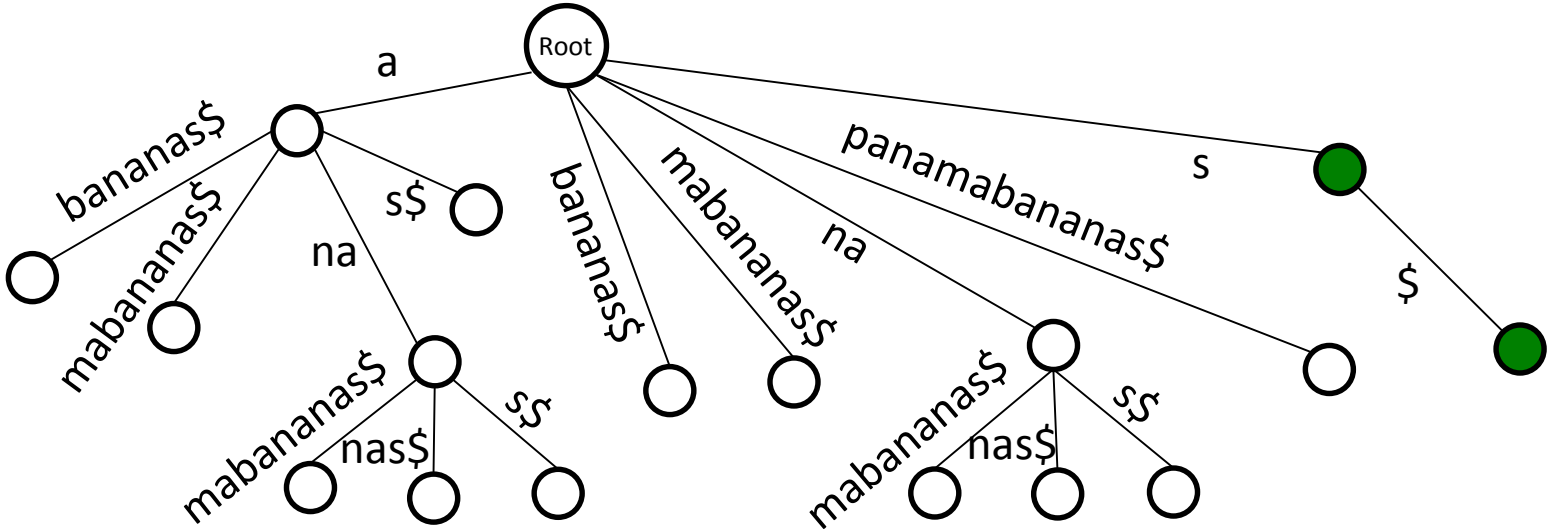
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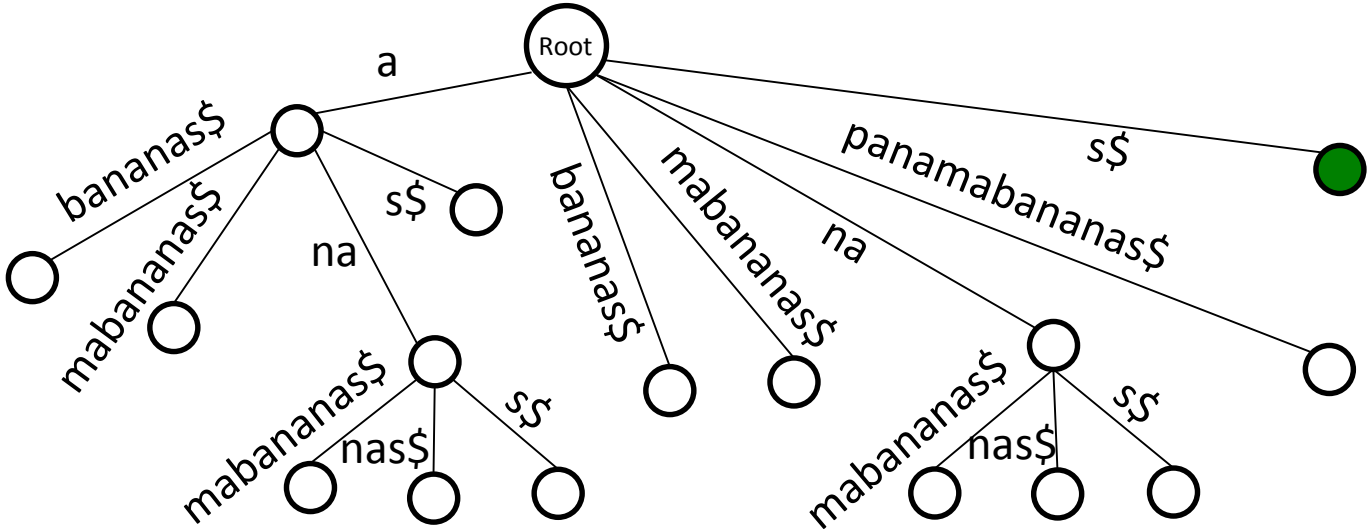
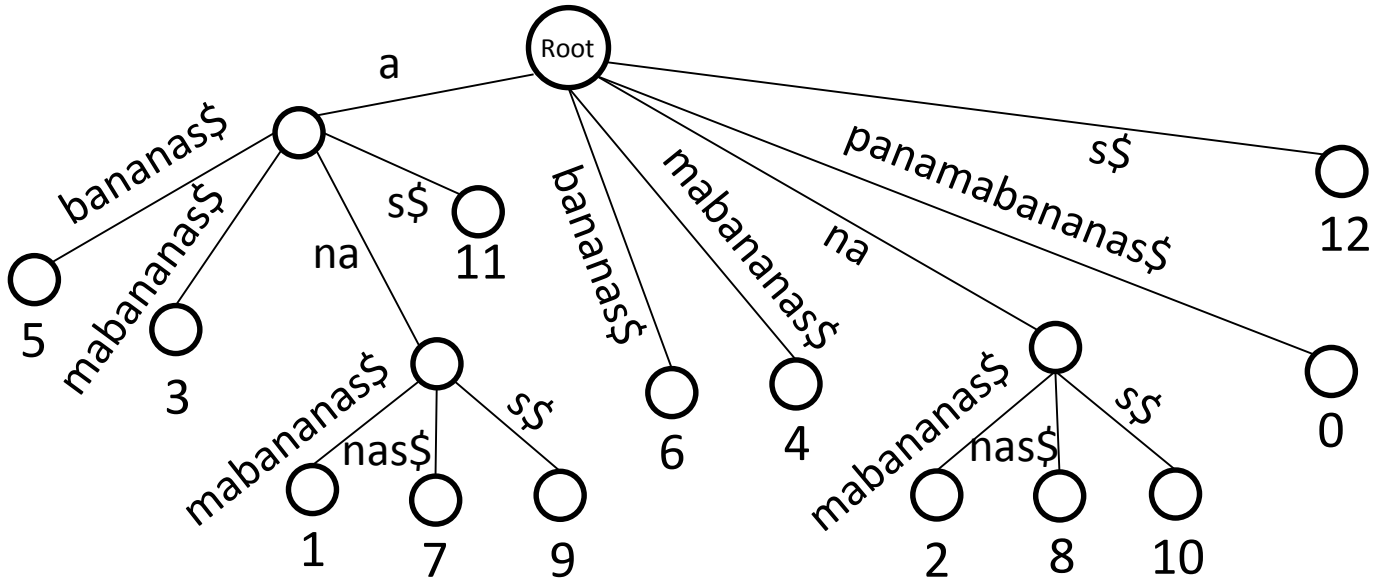
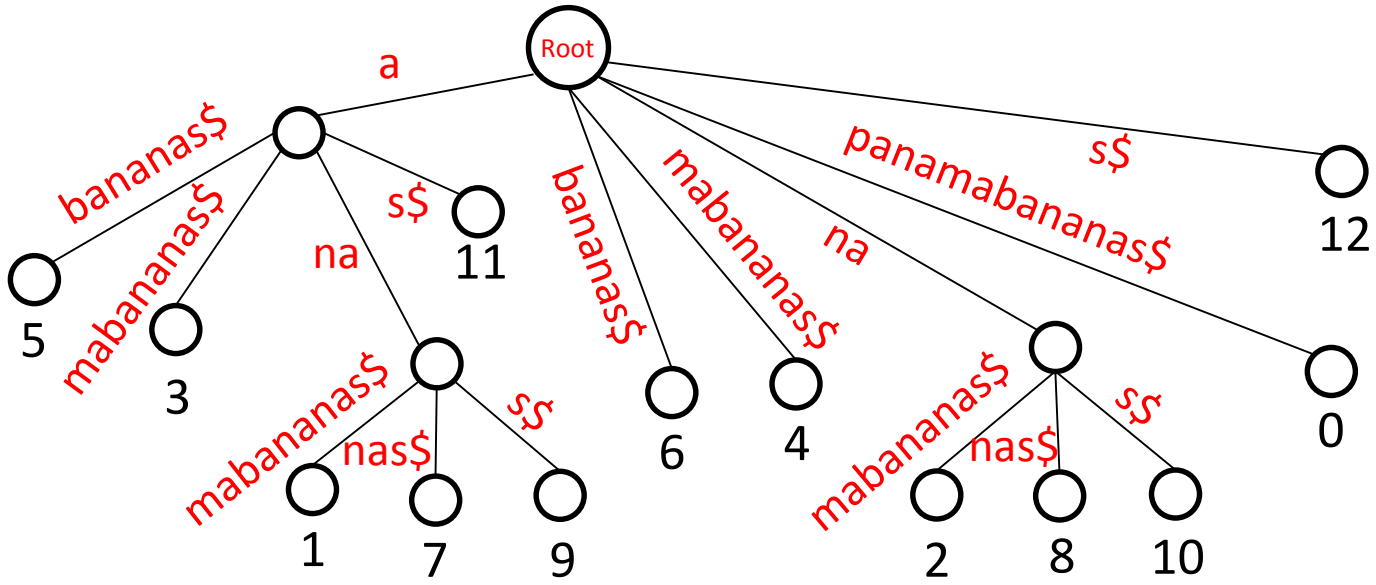


SuffixTree(*Text*)



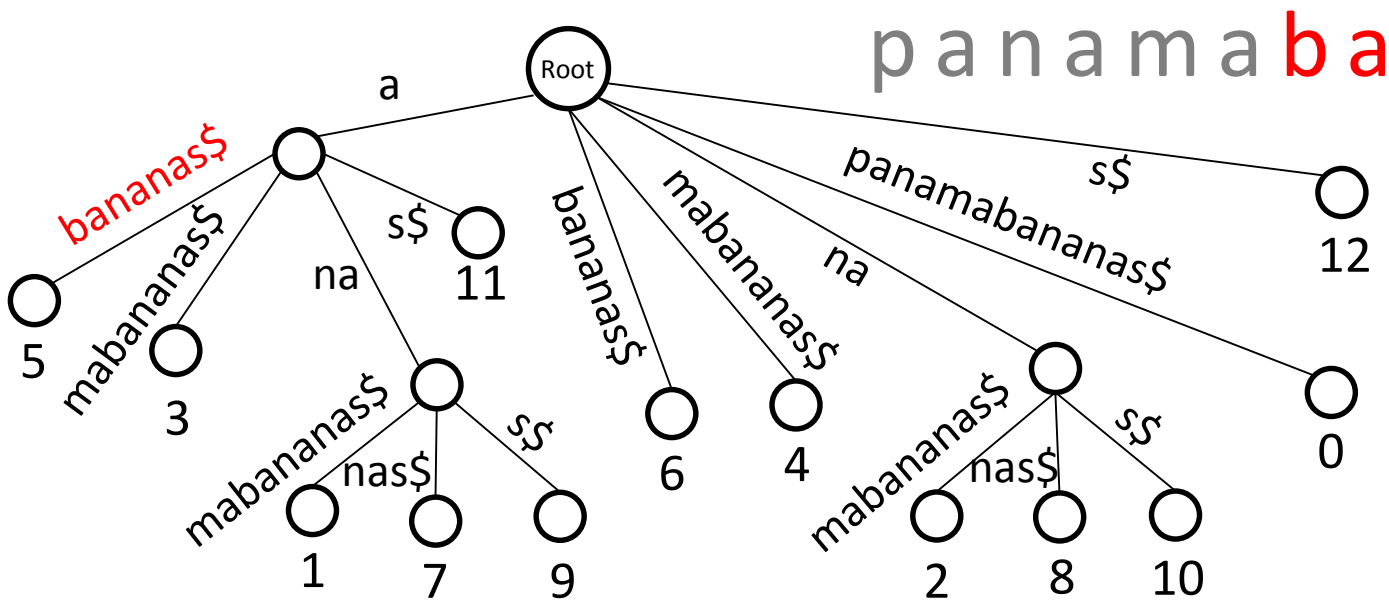
Since each suffix adds one leaf and at most one internal vertex to the suffix tree:

- # vertices < 2|*Text*|
- memory footprint of the suffix tree: O(|*Text*|)



Since each suffix adds one leaf and at most one internal vertex to the suffix tree:

- # vertices < 2|*Text*|
- memory footprint of the suffix tree: O(|*Text*|)
- **Cheating!!!** - how do we store all edge labels?

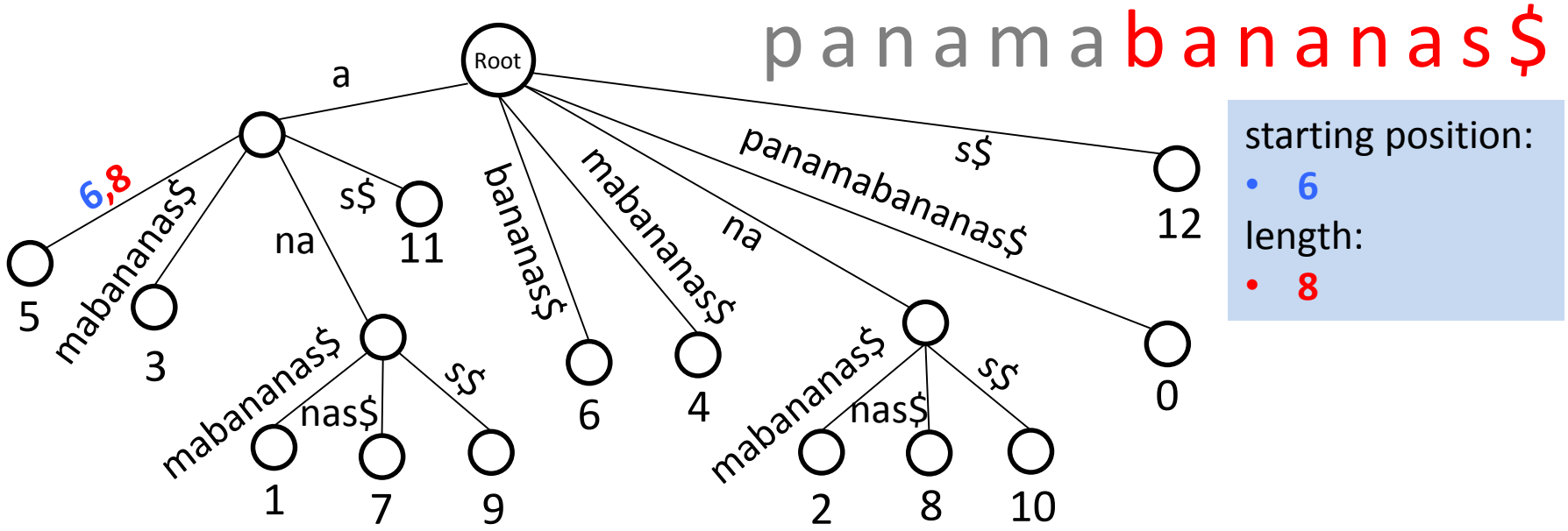


starting position:
- 6

length:
- 8

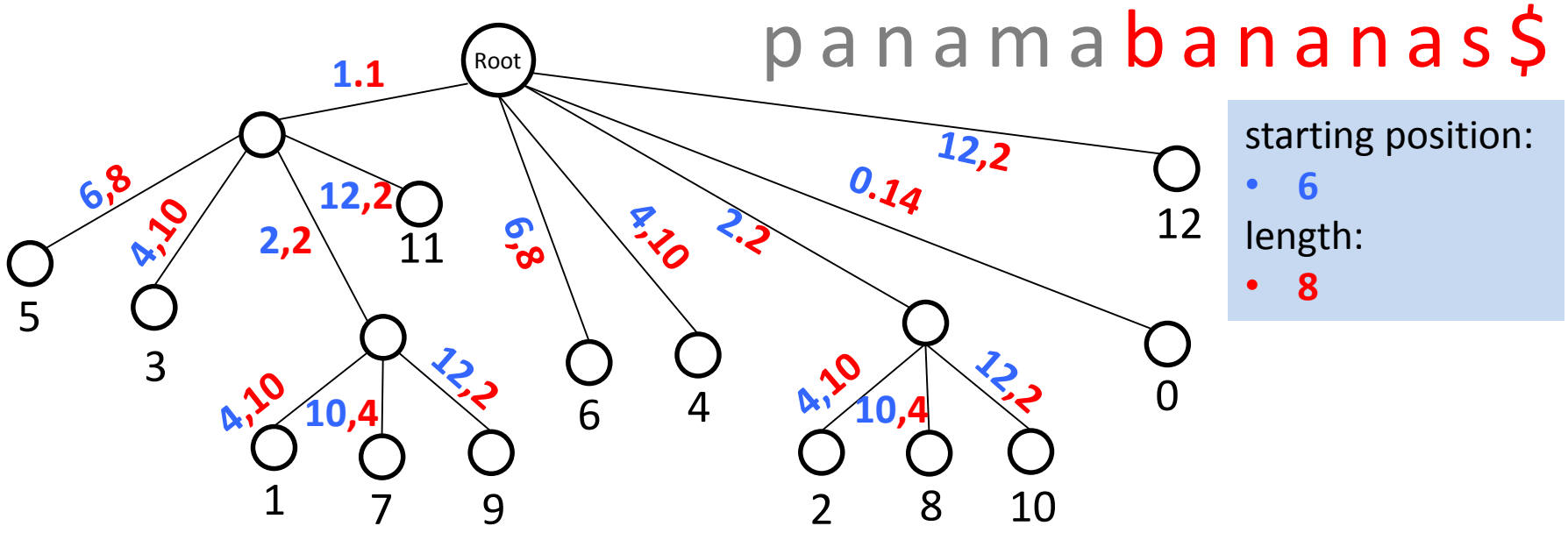
Since each suffix adds one leaf and at most one internal vertex to the suffix tree:

- # vertices < 2|*Text*|
- memory footprint of the suffix tree: O(|*Text*|)
- **Cheating!!!** - how do we store all edge labels?



Since each suffix adds one leaf and at most one internal vertex to the suffix tree:

- # vertices < 2|*Text*|
- memory footprint of the suffix tree: O(|*Text*|)
- storing edge labels



Since each suffix adds one leaf and at most one internal vertex to the suffix tree:

- # vertices < 2|*Text*|
- memory footprint of the suffix tree: O(|*Text*|)
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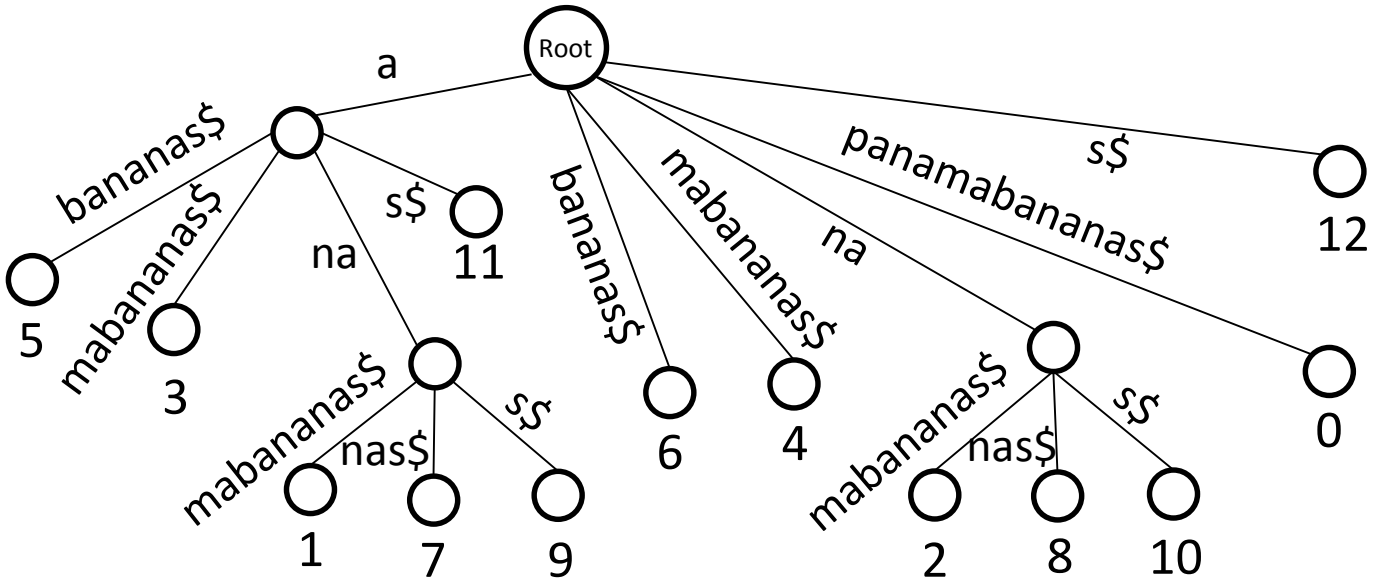

Why did we bother to add "**$**" to "panamabananas"?

- to make sure that each suffix corresponds to a leaf

Why do we want to make sure that each suffix correspond to a leaf?

- construct suffix tree for "papa"(without adding "$") and compare it with the suffix tree for "papa$"

Constructing Suffix Tree: **Naive Approach**

- **Quadratic** runtime:
  - $O(|Text|^2)$

$O(|Genome| + |Patterns|)$ to find pattern matches

Constructing Suffix Tree: **Linear-Time Algorithm**

- **Linear** runtime (for a constant-size alphabet):
  - O(|*Text*|)

Linear-time algorithm (Weiner, 1973) was simplified by Ukkonen (1995) but it is still too complex to cover in this course

Big Secret of the Big O Notation

- Suffix trees enable fast **Exact** Multiple Pattern Matching:
  - Runtime: O(|*Text*| + |*Patterns*|)
  - Memory: O(|*Text*|)
- However, big-O notation hides constants!
  - suffix tree algorithms has large memory footprint ~ 20•|*Text*| for long texts like human genome
- We want to find mutations!
  - it is unclear how to develop fast **Approximate** Multiple Pattern Matching using suffix trees