

Exact Matching : Techniques, Data Structures, Algorithms & Applications

Motivation:

Inexact/approximate match computing is time consuming, esp. for large scale data sets.

Exact Match detection can be used as a filter (pre-condition check)

Types of exact matches — Fixed-length
— variable-length

Data Structures for Exact Matches:

- Lookup table
- PATRICIA tree
- Suffix Tree, suffix array + LCP array
- compacted trie

Lookup Tables

Good for detection of small, fixed-length exact matches

e.g.; find all substrings of length 10 shared in common among a collection of strings.

Definition:

Let $\Sigma \leftarrow$ alphabet

$s \leftarrow$ input string of length n

$w \leftarrow$ user-defined parameter for fixed-length match

Given $\{s, \Sigma, w\}$ as input, a lookup table for s is ~~a~~ a table/record of all positions that map to in s

all possible substrings of length w .

e.g.; $w = 2 \Rightarrow$ there are $4^2 = 16$ possible strings; assuming $\Sigma = \{a, c, g, t\}$

Index: Table T

0	AA	
1	AC	$\rightarrow 1$
2	AG	$\rightarrow 4 \rightarrow 7$
3	AT	
4	CA	$\rightarrow 3$
5	CC	$\rightarrow 2$
6	CG	
7	CT	
8	GA	
9	GC	
10	GG	
11	GT	$\rightarrow 5 \rightarrow 8$
12	TA	$\rightarrow 6$
13	TC	$\rightarrow 9$
14	TG	
15	TT	

Let

$S = a \overbrace{c}^1 \overbrace{cag}^{2,3,4} t \overbrace{agt}^{5,6,7} c$

List of w -mers in s :

Pos#

ac	$\rightarrow 1$
cc	$\rightarrow 2$
ca	$\rightarrow 3$
ag	$\rightarrow 4$
gt	$\rightarrow 5$
ta	$\rightarrow 6$
ag	$\rightarrow 7$
gt	$\rightarrow 8$
tc	$\rightarrow 9$

Purpose of a lookup table:

Locations in S that share the same substring ~~sub~~ of length w , will be grouped together in the table.

Lookup Table Construction Algorithm:

- 0) Initialize lookup table T with null pointers
- 1) Slide a window of length w on S
- 2) For each window, length s_i be the substring
i.e.; $s_i = S[i..i+w-1]$
- 3) $\text{index} \leftarrow \text{hash}(s_i)$
- 4) $T[\text{index}].\text{insert}(i)$;

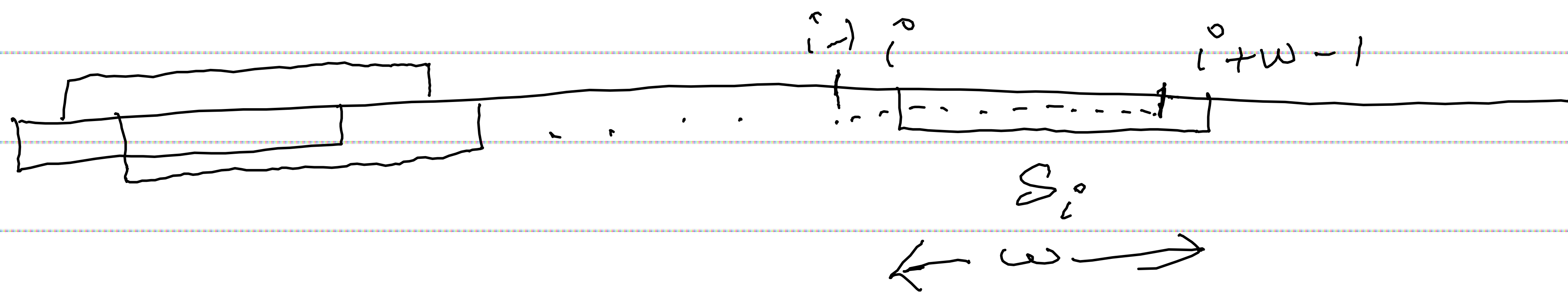
Key Properties of lookup Table:

1) space = $O(|\Sigma|^w)$ entries or pointers
+ $O(n)$ linked list entries

2) LT construction time = $O(\underbrace{|\Sigma|^w}_{\text{step (0)}} + \underbrace{n}_{\text{steps (1-4)}})$

(assuming $\text{hash}(s_i)$ can be computed in constant time)

How to compute $\text{hash}(s_i)$? (for all $s_i \in S$)



$\Sigma \Rightarrow$ integers

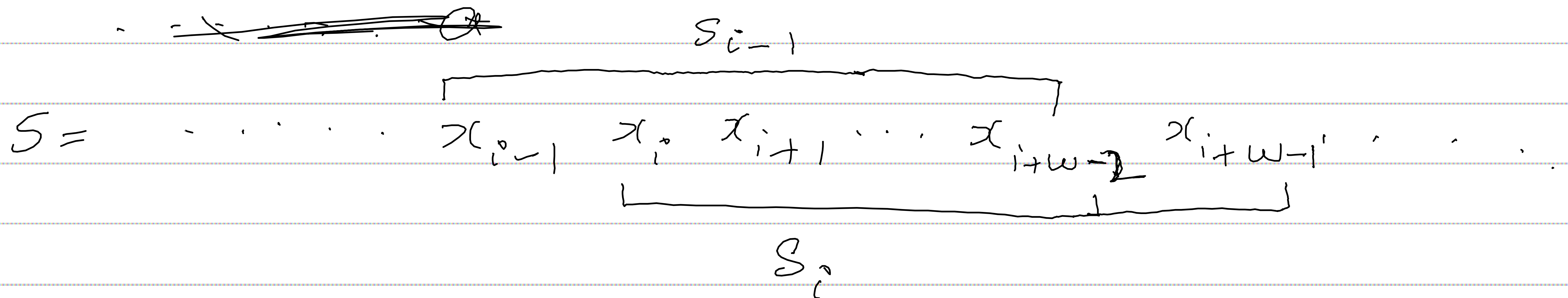
Lexicographic

$\left\{ \begin{array}{l} a \Rightarrow 0 \\ c \Rightarrow 1 \\ g \Rightarrow 2 \\ t \Rightarrow 3 \end{array} \right.$

Interpret each w -mer as a w -bit number with base $|\Sigma|$

$aa = 0$	$ca = 4$	$ga = 8$	$ta = 12$
$ac = 1$	$cc = 5$	$gc = 9$	$tc = 13$
$ag = 2$	$cg = 6$	$gg = 10$	$tg = 14$
$at = 3$	$ct = 7$	$gt = 11$	$tt = 15$

We can compute $\text{hash}(s_i)$ using the value $\text{hash}(s_{i-1})$



$$\text{hash}(s_i) = \left[\text{hash}(s_{i-1}) - h(x_{i-1}) \times |\Sigma|^{w-1} \right] \times |\Sigma| + h(x_{i+w-1})$$

Lookup Tables used heavily in BLAST
and a lot other applications.

Practical limitations:

→ Cannot scale for large values of w

e.g. ~~was~~ for DNA alphabet,

$$w = 10 \Rightarrow 4^{10} \Rightarrow \approx \text{~~1000~~} 10^6 \text{ entries}$$

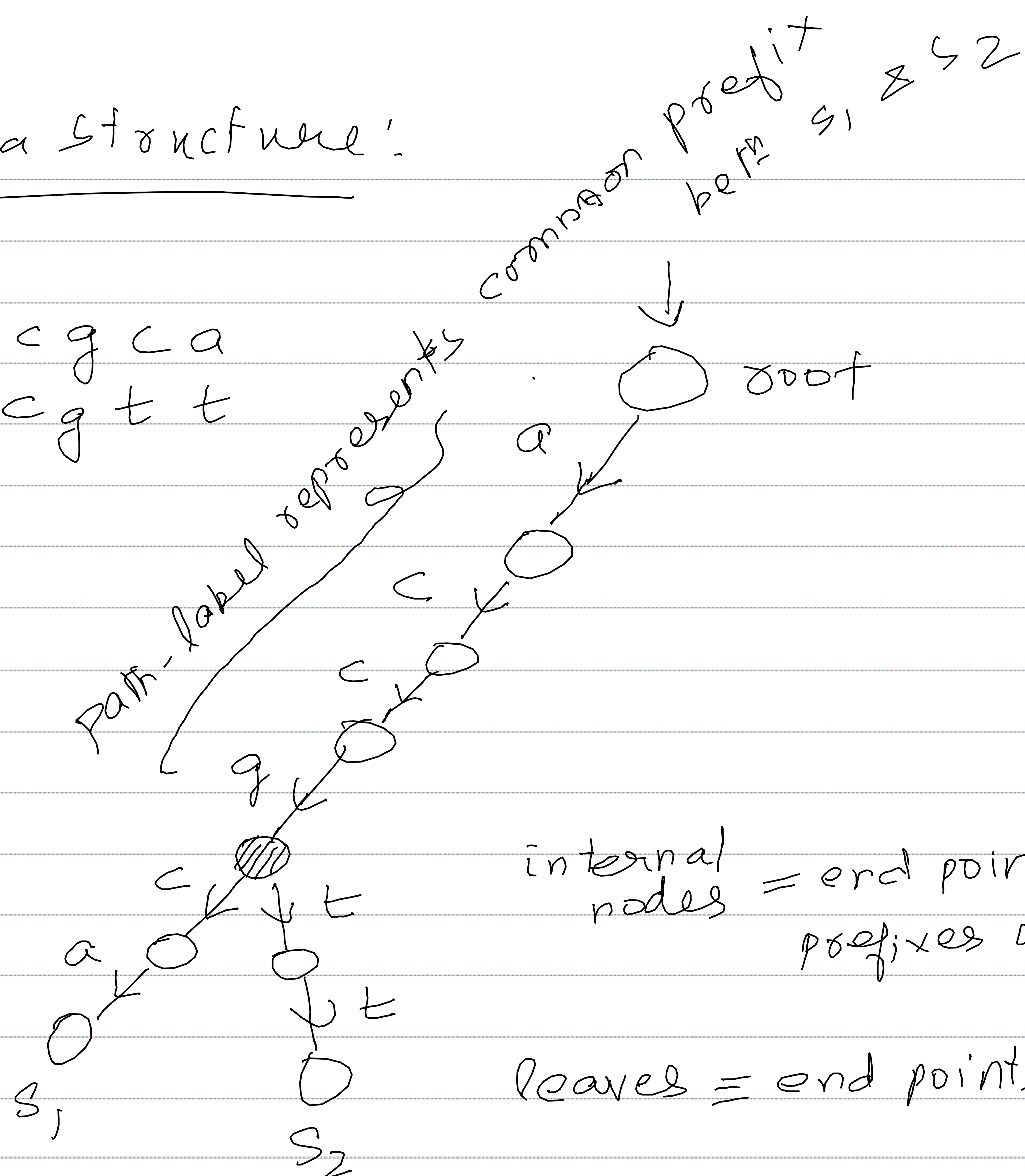
$$w = 15 \Rightarrow 4^{15} \Rightarrow 10^9 \text{ entries}$$

$$w = 20 \Rightarrow 4^{20} \Rightarrow 2^{40} \text{ or } 10^{12} \text{ entries!}$$

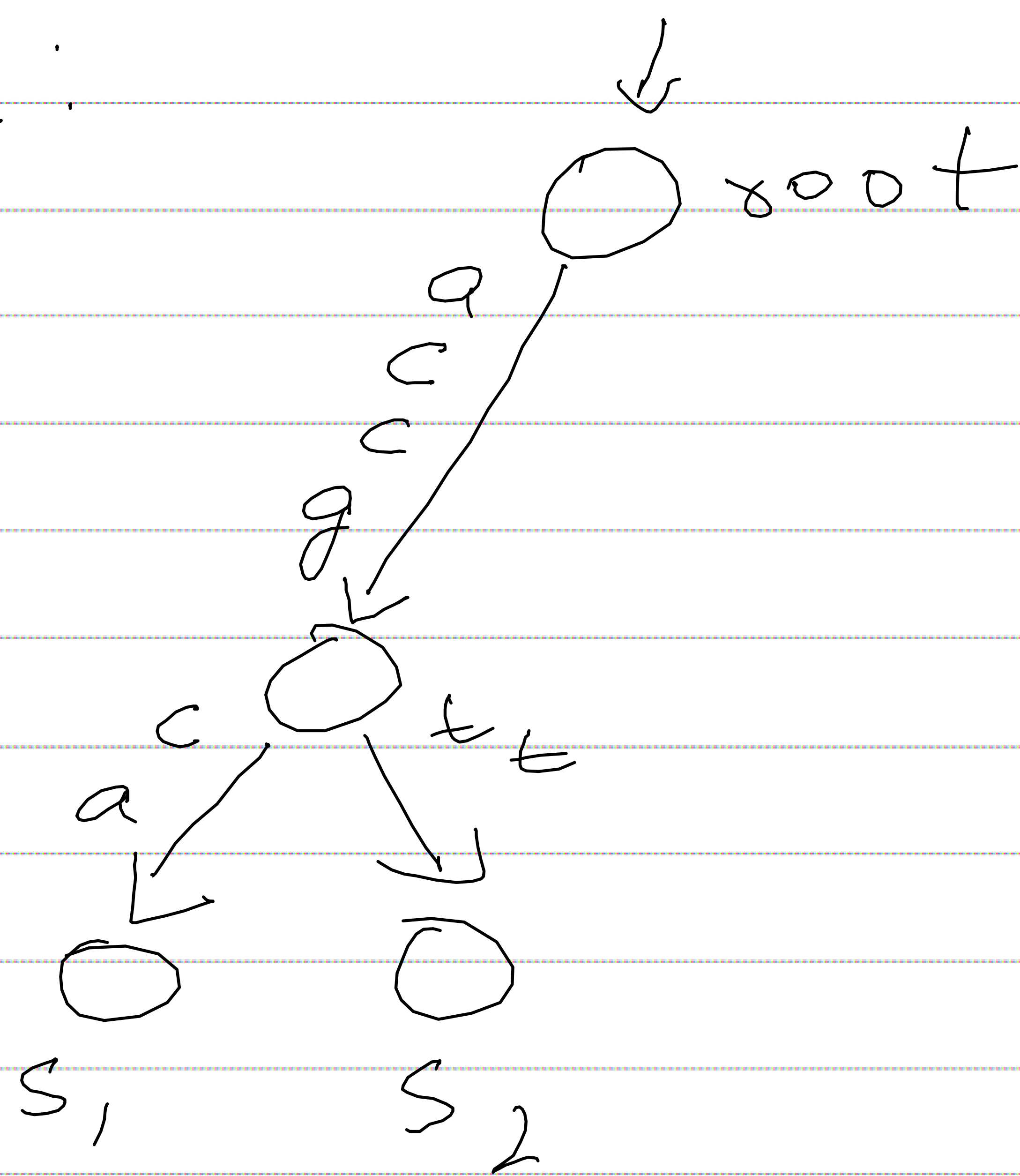
Trie data structure:

$S_1 = a c c g c a$

$S_2 = a c c g t t$



Compacted Trie:



(Morris, 1968)

PATRICIA Tree $\equiv$ compacted trie of an arbitrary number of input strings.

~~Practical~~ Practical Appli.

"Practical Algorithm to Retrieve Information Coded in Alphabetic"