Ch32 String Matching

- Introduction
- Naïve Algorithm
- Rabin-Karp Algorithm
- String Matching using Finite Automata
- Knuth-Morris-Pratt (KMP) Algorithm
- Indexing Method: BWT (Suppl.)

To various sources, including Profs. Ananth Grama, Mehmet Koyuturk, Michael Raymer, Wiki sources (pictures), and other noted attributions

Introduction

- What is string matching?
 - Finding all occurrences of a pattern in a given text (or body of text).
- Many applications:
 - While using editor/word processor/browser.
 - Login name & password checking.
 - Virus detection.
 - Header analysis in data communications.
 - DNA sequence analysis.

History of String Search

- The brute force algorithm
 - invented in the dawn of computer history.
 - re-invented many times, still common.
- Knuth & Pratt invented a better one in 1970
 - published 1976 as "Knuth-Morris-Pratt".
- Boyer & Moore found a better one before 1976
 - Published 1977.
- •Karp & Rabin found a "better" one in 1980
 - Published 1987.

Algorithm	Preprocessing Time	Matching Time
Naive	0	O((n-m+1)m)
Rabin-Karp	$\Theta(m)$	O((n-m+1)m)
Finite Automaton	$O(m \Sigma)$	$\Theta(n)$
Knuth-Morris-Pratt	$\Theta(m)$	$\Theta(n)$
Boyer-Moore	$\Theta(m)$	$\Theta(n)$

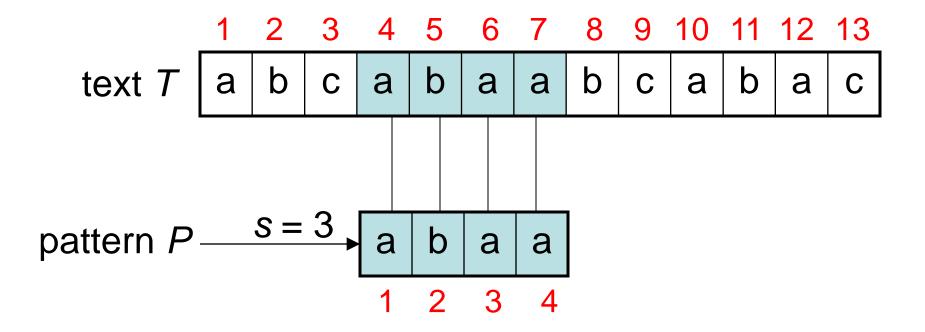
String-Matching Problem

- The text is in an array T [1..n] of length n.
- The pattern is in an array P [1..m] of length m.
- Elements of T and P are characters from a *finite alphabet* Σ .
 - E.g., $\Sigma = \{0,1\}$ or $\Sigma = \{a, b, ..., z\}$.
- Usually T and P are called strings of characters.

String-Matching Problem ...contd

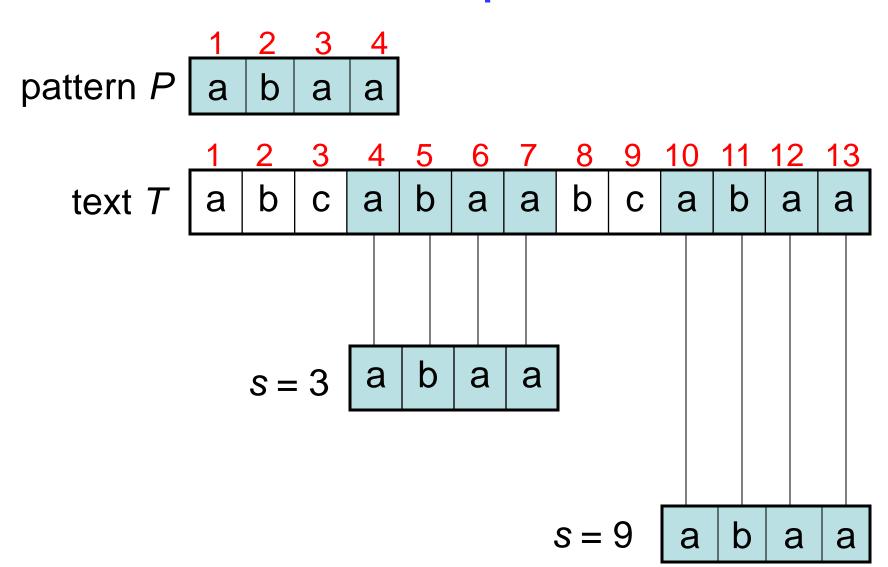
- We say that pattern P occurs with shift s in text T if:
 - a) $0 \le s \le n-m$ and
 - b) T[(s+1)..(s+m)] = P[1..m].
- If P occurs with shift s in T, then s is a
 valid shift, otherwise s is an invalid shift.
- String-matching problem: finding all valid shifts for a given T and P.

Example 1



shift s = 3 is a valid shift $(n=13, m=4 \text{ and } 0 \le s \le n-m \text{ holds})$

Example 2



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Naïve String-Matching Algorithm

Input: Text strings T[1..n] and P[1..m].

Result: All valid shifts displayed.

NA $\ddot{\mathbf{I}}$ VE-STRING-MATCHER (T, P)

```
n \leftarrow length[T]

m \leftarrow length[P]

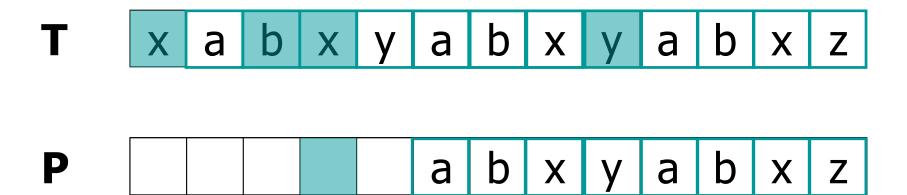
for s \leftarrow 0 to n-m

if P[1..m] = T[(s+1)..(s+m)]

print "pattern occurs with shift" s
```

Example

P="abxyabxz" and T="xabxyabxyabxz"



Worst-case Analysis

- There are m comparisons for each shift in the worst case.
- There are n-m+1 shifts.
- So, the worst-case running time is $\Theta((n-m+1)m)$.
- Na ve method is inefficient because information from a shift is not used again.

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Rabin-Karp Algorithm

- Has a worst-case running time of O((n-m+1)m) but average-case is O(n+m).
 - Also works well in practice.
- Based on number-theoretic notion of modular equivalence.
- We assume that $\Sigma = \{0,1, 2, ..., 9\}$, i.e., each character is a decimal digit.
 - In general, use radix-d where $d = |\Sigma|$.

Modular Equivalence

- If $(a \mod n) = (b \mod n)$, then we say "a is equivalent to b, modulo n".
- Denoted by $a \equiv b \pmod{n}$.

- That is, $a \equiv b$ (mod n) if a and b have the same remainder when divided by n.
 - E.g., $23 \equiv 37 \equiv -19 \pmod{7}$.

Rabin-Karp Approach

- We can view a string of k characters (digits) as a length-k decimal number.
 - E.g., the string "31425" corresponds to the decimal number 31,425.
- Given a pattern P [1..m], let p denote the corresponding decimal value.
- Given a text T[1..n], let t_s denote the decimal value of the length-m substring T[(s+1)..(s+m)] for s=0,1,...,(n-m).

Rabin-Karp Approach ...contd

- $t_s = p \text{ iff } T[(s+1)..(s+m)] = P[1..m].$
- s is a valid shift iff $t_s = p$.
- p can be computed in O(m) time.
 - p = P[m] + 10 (P[m-1] + 10 (P[m-2]+...)).
- t_0 can similarly be computed in O(m) time.
- Other t₁, t₂,..., t_{n-m} can be computed in O(n-m) time since t_{s+1} can be computed from t_s in constant time.

Rabin-Karp Approach ...contd

- $t_{s+1} = 10(t_s 10^{m-1} \cdot T[s+1]) + T[s+m+1]$
 - E.g., if $T=\{...,3,1,4,1,5,2,...\}$, m=5 and $t_s=31,415$, then $t_{s+1}=10(31415-10000\cdot3)+2$
- We can compute p, t_0 , t_1 , t_2 ,..., t_{n-m} in O(n+m) time.

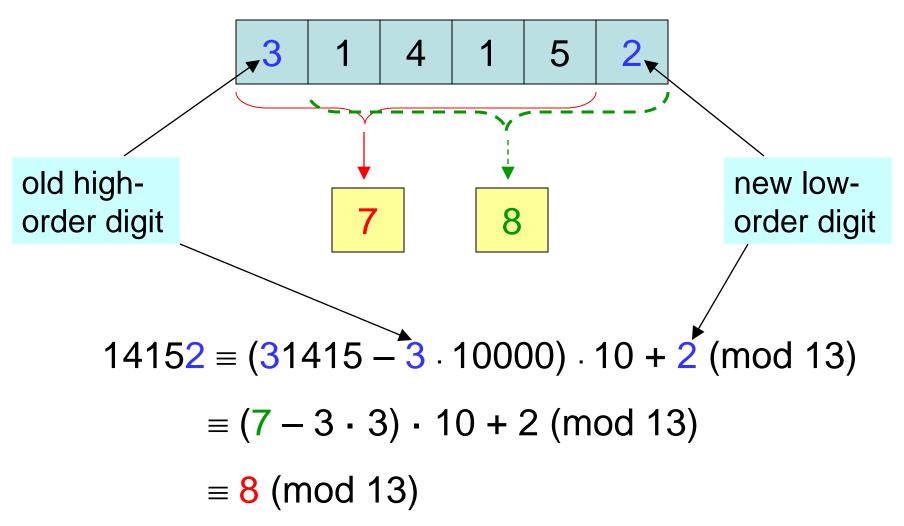
- But...a problem: this is assuming p and t_s are small numbers.
 - They may be too large to work with easily.

Rabin-Karp Approach ...contd

- Solution: we can use modular arithmetic with a suitable modulus, q.
 - E.g., $t_{s+1} \equiv 10(t_s ...) + T[s+m+1] \pmod{q}$.

- q is chosen as a small prime number, e.g., 13 for radix 10.
 - Generally, if the radix is d, then dq should fit within one computer word.

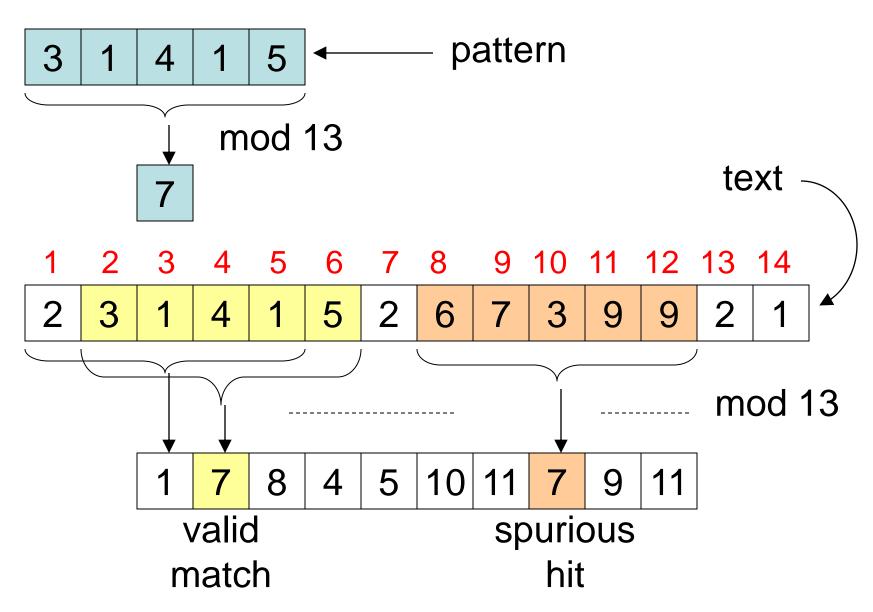
How values modulo 13 are computed



Problem of Spurious Hits

- $t_s \equiv p \pmod{q}$ does not imply that $t_s = p$.
 - Modular equivalence does not necessarily mean that two integers are equal.
- A case in which t_s ≡ p (mod q) when t_s ≠ p is called a spurious hit.
- On the other hand, if two integers are not modular equivalent, then they cannot be equal.

Example



Rabin-Karp Algorithm

- Basic structure like the na ve algorithm, but uses modular arithmetic as described.
- For each *hit*, i.e., for each s where $t_s \equiv p$ (mod q), verify character by character. whether s is a valid shift or a spurious hit
- In the worst case, every shift is verified.
 - Running time can be shown as O((n-m+1)m).
- Average-case running time is O(n+m).

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Finite Automata

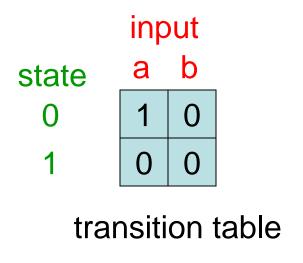
- A finite automaton M is a 5-tuple (Q, q_0 , A, Σ , δ), where
 - Q is a finite set of states.
 - $-q_0 \in Q$ is the start state.
 - $A \subseteq Q$ is a set of accepting states.
 - $-\sum$ is a finite *input alphabet*.
 - δ is the *transition function* that gives the next state for a given current state and input.

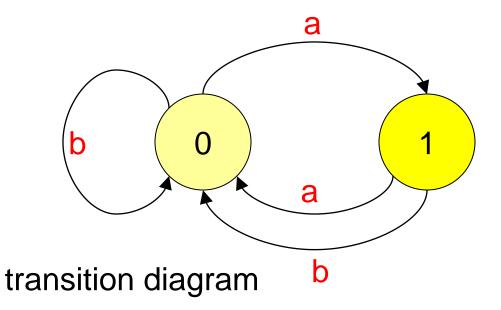
How a Finite Automaton Works

- The finite automaton M begins in state $q_{0.}$
- Reads characters from Σ one at a time.
- If M is in state q and reads input character a, M moves to state $\delta(q,a)$.
- If its current state q is in A, M is said to have accepted the string read so far.
- An input string that is not accepted is said to be rejected.

Example

- $Q = \{0,1\}, q_0 = 0, A = \{1\}, \Sigma = \{a, b\}.$
- $\delta(q,a)$ shown in the transition table/diagram.
- This accepts strings that end in an odd number of a's; e.g., abbaaa is accepted, aa is rejected.





String-Matching Automata

- Given the pattern P [1..m], build a finite automaton M.
 - The state set is $Q=\{0, 1, 2, ..., m\}$.
 - The start state is 0.
 - The only accepting state is m.

• Time to build M can be large if Σ is large.

String-Matching Automata ...contd

Scan the text string T[1..n] to find all occurrences of the pattern P[1..m].

- String matching is efficient: $\Theta(n)$.
 - Each character is examined exactly once.
 - Constant time for each character.
- But ...time to compute δ is $O(m |\Sigma|)$.
 - − δ Has $O(m |\Sigma|)$ entries.

Algorithm

Input: Text string T[1..n], δ and m

Result: All valid shifts displayed

FINITE-AUTOMATON-MATCHER (T, m, δ)

```
n \leftarrow length[T]

q \leftarrow 0

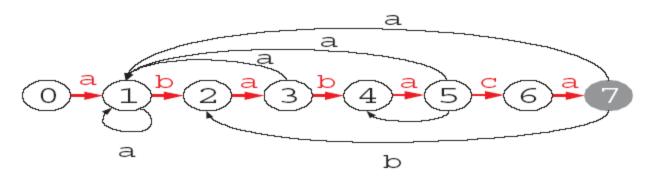
for i \leftarrow 1 to n

q \leftarrow \delta (q, T[i])

if q = m

print "pattern occurs with shift" i-m
```

Example



state	a	b	c	P
0	1	0	0	a
1	1	2	0	b
2	3	0	0	a
3	1	4	0	b
4	5	0	0	a
5	1	4	6	c
6	7	0	0	a
7	1	2	Ο	

$$i$$
 — 1 2 3 4 5 6 7 8 9 10 11 $T[i]$ — a b a b a b a c a b a $\phi(T_i)$ 0 1 2 3 4 5 4 5 6 7 2 3

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Knuth-Morris-Pratt (KMP) Method

- Avoids computing δ (transition function).
- Instead computes a *prefix function* π in O(m) time.
 - π has only m entries.

- Prefix function stores info about how the pattern matches against shifts of itself.
 - Can avoid testing useless shifts.

Terminology/Notations

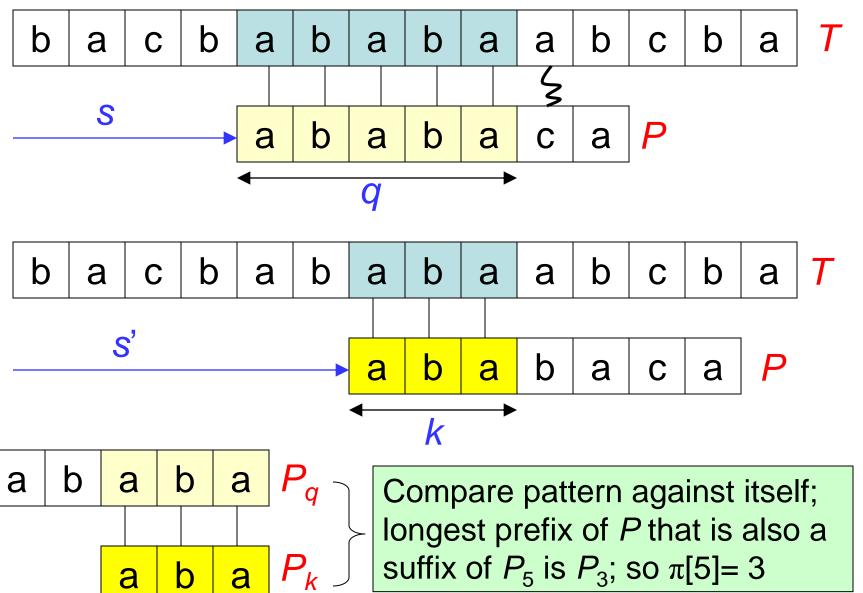
- String w is a prefix of string x, if x=wy for some string y (e.g., "srilan" of "srilanka").
- String w is a suffix of string x, if x=yw for some string y (e.g., "anka" of "srilanka").
- The k-character prefix of the pattern P [1..m] denoted by P_k
 - E.g., $P_0 = \varepsilon$, $P_m = P = P [1..m]$.

Prefix Function for a Pattern

• Given that pattern prefix P[1..q] matches text characters T[(s+1)..(s+q)], what is the least shift s' > s such that P[1..k] = T[(s'+1)..(s'+k)] where s'+k=s+q?

- At the new shift s', no need to compare the first k characters of P with corresponding characters of T.
 - Since we know that they match.

Prefix Function: Example 1



Prefix Function: Example 2

i	1	2	3	4	5	6	7	8	9	10
P[i]	а	b	а	b	а	b	а	b	С	а
$\pi[i]$	0	0	1	2	3	4	5	6	0	1

 $\pi[q] = \max \{ k \mid k < q \text{ and } P_k \text{ is a suffix of } P_q \}$

Illustration: given a String 'S' and pattern 'p' as follows:

S bacbabababacaca

p a b a b a c a

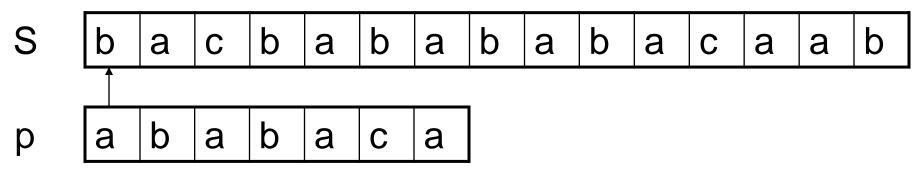
Let us execute the KMP algorithm to find whether 'p' occurs in 'S'.

For 'p' the prefix function, Π was computed previously and is as follows:

q	1	2	3	4	5	6	7
р	а	b	а	b	а	С	а
П	0	0	1	2	3	0	1

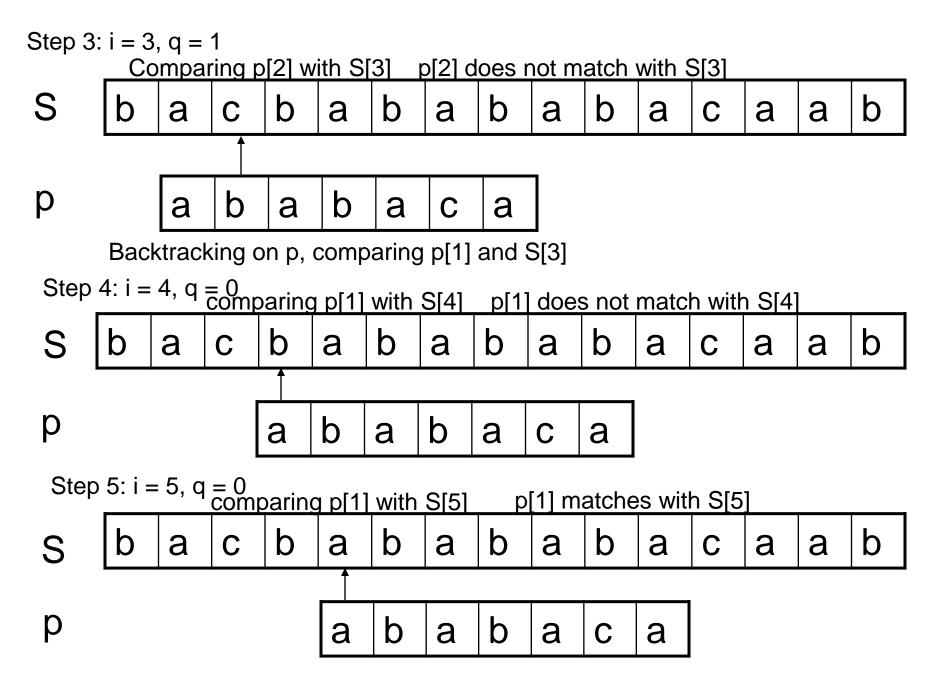
Initially:
$$n = size of S = 15$$
; $m = size of p = 7$

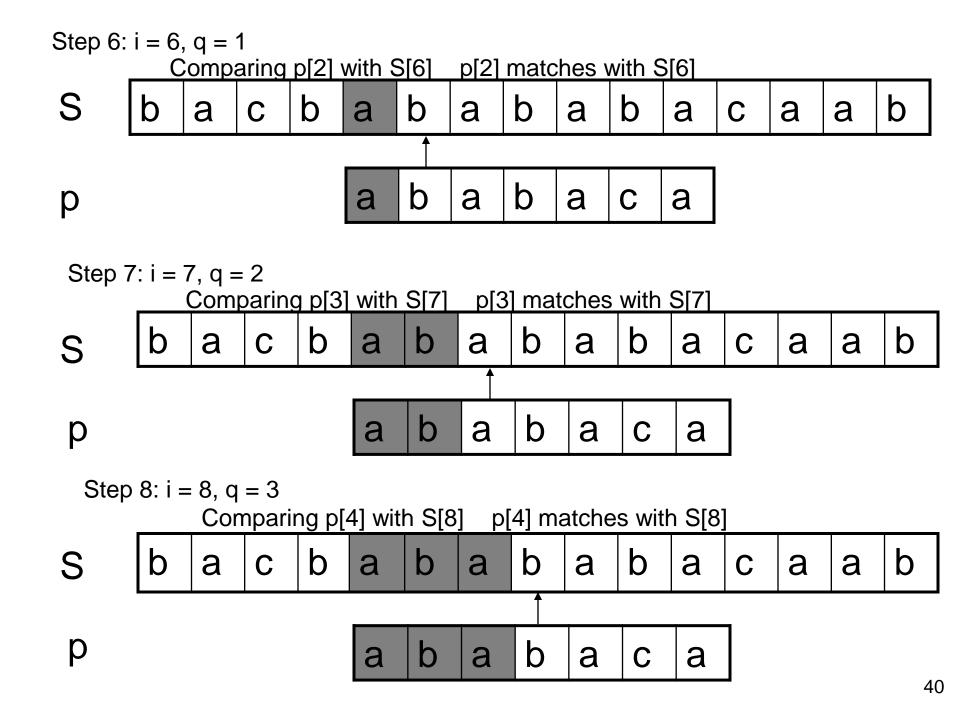
Step 1:
$$i = 1$$
, $q = 0$
comparing p[1] with S[1]



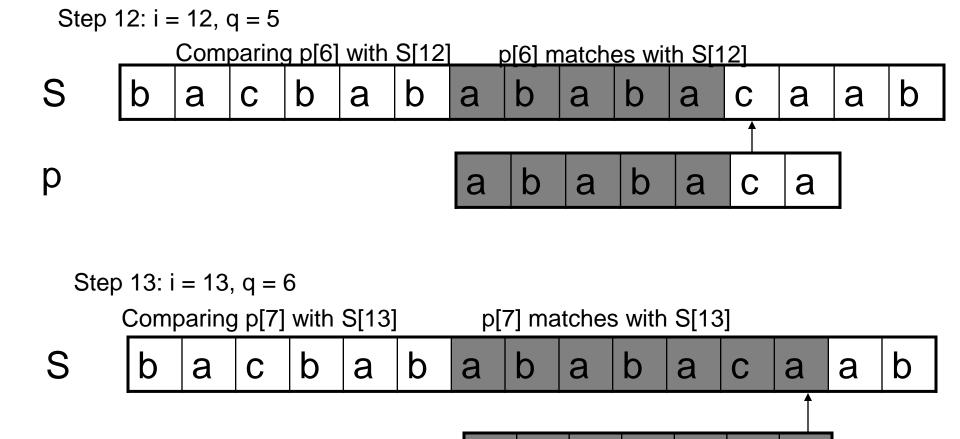
P[1] does not match with S[1]. 'p' will be shifted one position to the right.

P[1] matches S[2]. Since there is a match, p is not shifted.





Step 9: i = 9, q = 4Comparing p[5] with S[9] p[5] matches with S[9] S a b a b b a a p b b a a a a Step 10: i = 10, q = 5p[6] doesn't match with S[10] Comparing p[6] with S[10] b b b b a C a a a b S a C b b a a a p a Backtracking on p, comparing p[4] with S[10] because after mismatch $q = \Pi[5] = 3$ Step 11: i = 11, q = 4Comparing p[5] with S[11] p[5] matches with S[11] b a b C D b a a a a S b a a a 41



Pattern 'p' has been found to completely occur in string 'S'. The total number of shifts that took place for the match to be found are: i - m = 13 - 7 = 6 shifts.

b

a

a

a

p

Knuth-Morris-Pratt (KMP) Algorithm

- Information stored in prefix function
 - Can speed up both the naïve algorithm and the finite-automaton matcher.
- KMP Algorithm
 - 2 parts: KMP-MATCHER, PREFIX.
- Running time
 - PREFIX takes O(m).
 - KMP-MATCHER takes O(m+n).

Boyer-Moore Algorithm

- Published in 1977.
- The longer the pattern is, the faster it works.
- Starts from the end of pattern, while KMP starts from the beginning.
- Works best for character string, while KMP works best for binary string.
- KMP and Boyer-Moore
 - Preprocessing existing patterns.
 - Searching patterns in input strings.

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Short read mapping

Input:

- A reference genome.
- A collection of many 25-100bp reads.
- User-specified parameters (best or all mapping...).

Output:

One or more genomic coordinates for each read.

Multiple mapping

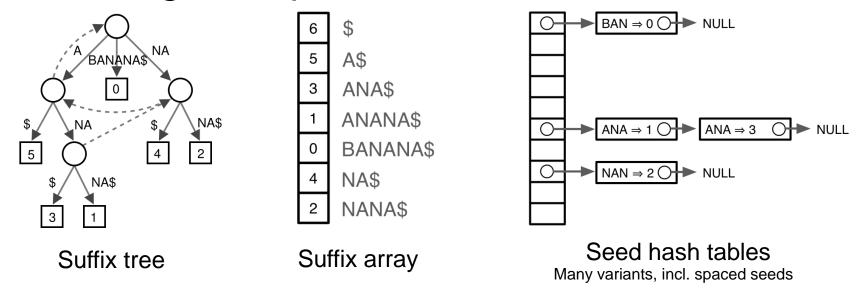
Mapping Reads Review

- Hash Table (Lookup table): exact match
 - Fast, but only for with fixed length. $[O(\alpha(n)N), lookup time \alpha(n)]$
- Suffix Trees or Suffix Array: exact match
 - Can handle patterns with variable length. [O(mN)]
 - Constructing suffix array require at least $n\lceil \log_2 n \rceil$ bits of working space.
- Dynamic Programming (Smith Waterman): approximate match
 - Mathematically optimal solution for Indels (插入/删除).
 - Slow, needs filter out impossible positions in practice. [O(mnN)]
- FM-index with Burrows-Wheeler Transform: exact match
 - Fast for small alphabet. $[O(mN\log_2 \alpha), \alpha \text{ is the size of alphabet}]$
 - Memory efficient, total is less than 1.5GB for human genome.

Where *m* is the length of reads, *n* is the length of genome, *N* is the number of reads.

Indexing (1)

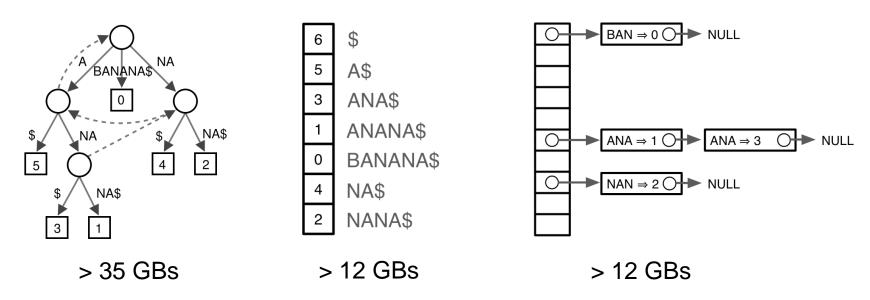
Indexing is required



Choice of index is key to performance.

Indexing (2)

Genome indices can be big. For human:

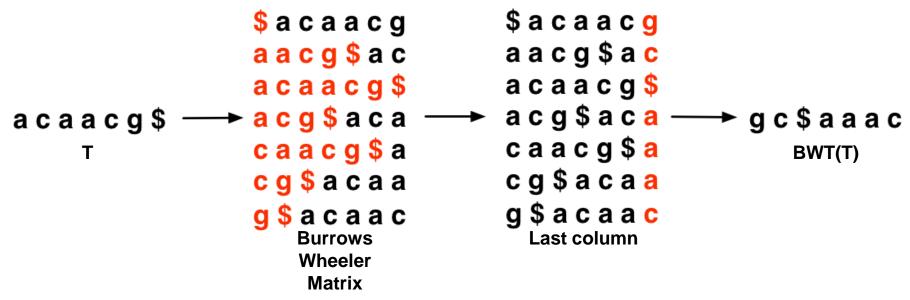


- Large indices necessitate painful compromises:
 - 1. Require big-memory machine
 - 2. Use secondary storage

- 3. Build new index each run
- 4. Subindex and do multiple passes

Building: From T to BWT(T)

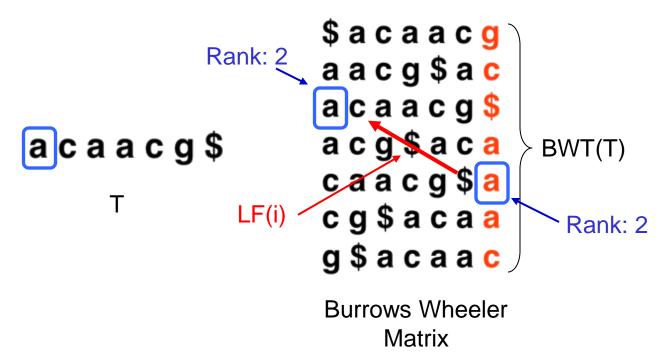
Reversible permutation used originally in compression.



- Once BWT(T) is built, all else shown here is discarded.
 - Matrix will be shown for illustration only.

LF Mapping of BWT

- Property that makes BWT(T) reversible is "LF Mapping".
 - Property: ith occurrence of a character in Last column is same text occurrence as the ith occurrence in First column.
 - E.g. LF(5)=3 is the map from last row to first row, where 5 is line# of last and 3 is line# of first for the same a of rank 2.



Recover: From BWT(T) to T

- To recreate T from BWT(T), repeatedly apply rule:
 - T = BWT[LF(i)] + T; j = LF(i).
 - Where LF(i) maps row i to row j whose first column character corresponds to j's last column per LF Mapping.

```
caacq
                                                             acaacq
                                        aacg
                             a c g
$acaacg
           $acaacg
                        $acaacg
                                    $acaacg
                                                $acaacg
                                                            $acaacg
                                                            aacg$ac
aacg$ac
            aacg$ / c
                        aacg$ac
                                    aacg$ac
                                                a eg sta c
            a c a a \sqrt{g}
acaacg$
                        acaacg$
                                    acaacg$
                                                acaacg$
                                                            a c a a 🧷
                                                acg$aca
acg$aca
            acg yaca
                       acg$aca
                                    a <del>cg $ a ≥</del> a
            caa/cg$a
                        caacg$a
caacg$a
                                    caatg$a
                                                caacg$a
cg$acaa
                        c <del>stack</del>a
                                    cg$acaa
                                                cg$acaa
                                                            cg$acaa
g $ a c a a c
                        q $ a c a a c
                                    g $ a c a a c
                                                q $ a c a a c
                                                            g $ a c a a c
```

Could be called "unpermute (解置换)" or "walk-left" algorithm.

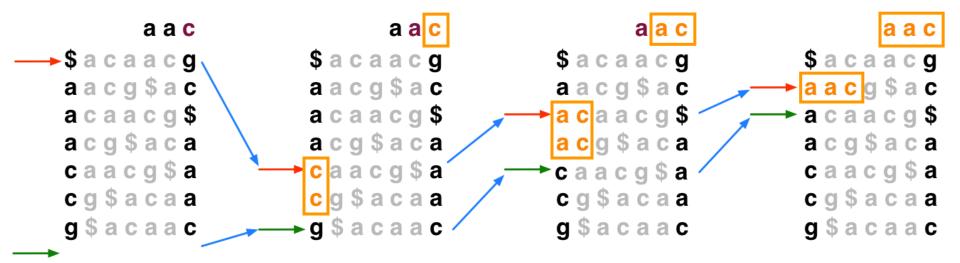
FM Index

Ferragina & Manzini propose "FM Index" based on BWT.

- Observed:
 - LF Mapping also allows exact matching within T.
 - LF(i) can be made fast with checkpointing.
 - ...and more (see FOCS paper).
- Ferragina P, Manzini G: Opportunistic data structures with applications. FOCS. IEEE Computer Society; 2000.
- Ferragina P, Manzini G: An experimental study of an opportunistic index. SIAM symposium on Discrete algorithms. Washington, D.C.; 2001.

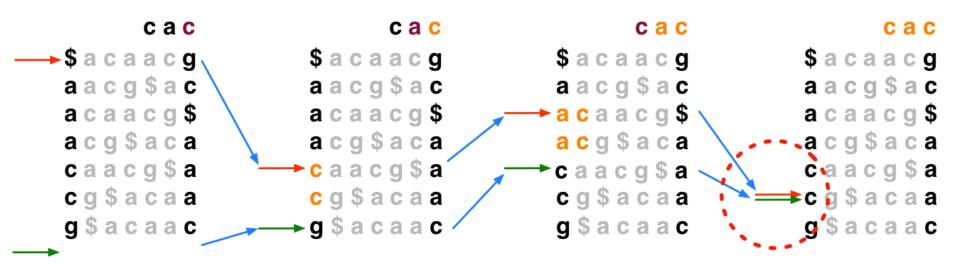
Searching with FM Index: Existed

- To match Q in T using BWT(T), repeatedly apply rule:
 - top = LF(top, qc) //also by sp;
 bot = LF(bot, qc) //also by ep
 - Where qc is the next character in Q (right-to-left) and LF(i, qc) maps row i to the row whose first column character corresponds to i's last column character as if it were qc.



 In progressive rounds, top & bot delimit the range of rows beginning with progressively longer suffixes of Q.

Searching with FM Index: Inexisted



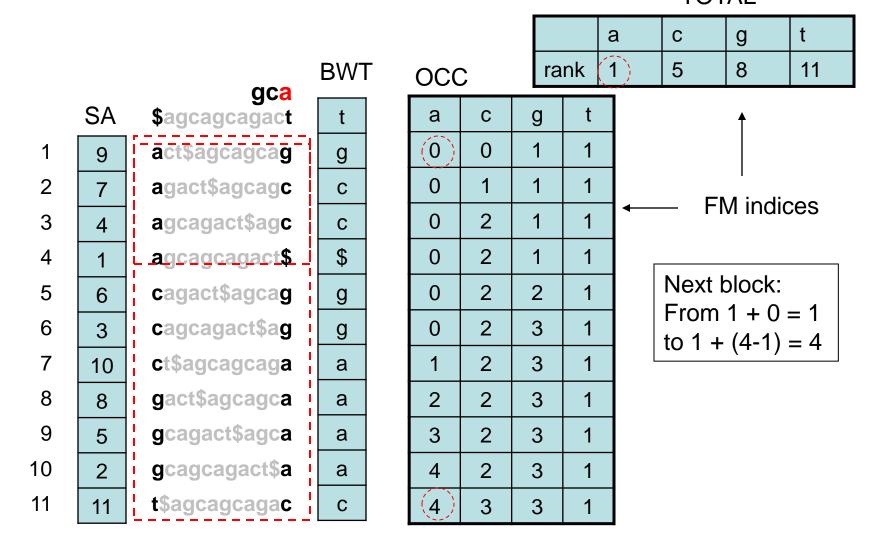
 If range becomes empty (top = bot) the query suffix (and therefore the query) does not occur in the text.

Key for efficient pattern matching: how to find the corresponding chars in the first column efficiently, in terms of both time and space.

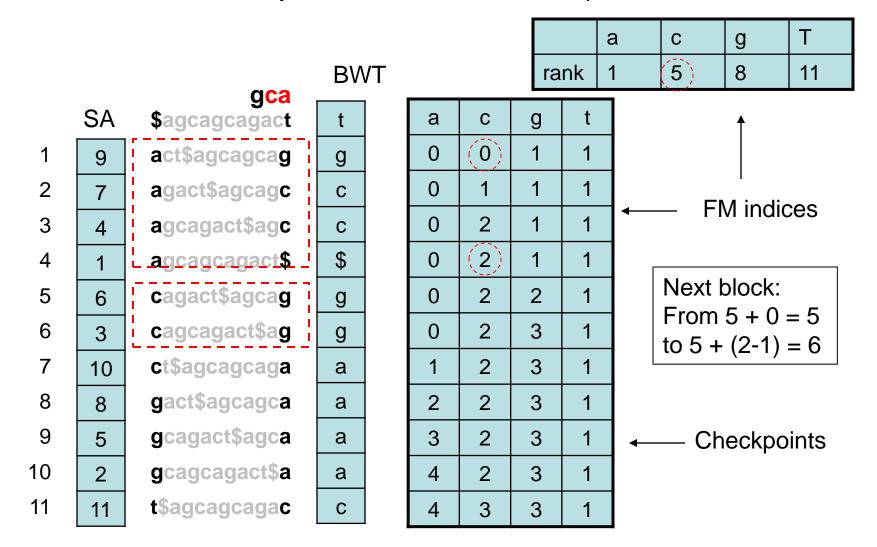
									а	С	g	Т	
			BW	/ T			ra	nk	1	5	8	11	
	SA	\$agcagcagact	t		а	С	g	t			†		
1	9	act\$agcagcag	g		0	0	1	1		←— FM indices			
2	7	agact\$agcagc	С		0	1	1	1					
3	4	agcagact\$agc	С		0	2	1	1					
4	1	agcagcagact\$	\$		0	2	1	1					
5	6	cagact\$agcag	g		0	2	2	1					
6	3	cagcagact\$ag	g		0	2	3	1					
7	10	ct\$agcagcaga	а		1	2	3	1					
8	8	gact\$agcagca	а		2	2	3	1					
9	5	gcagact\$agca	а		3	2	3	1		— Ch	eckpo	ints	
10	2	gcagcagact\$a	а		4	2	3	1					
11	11	t\$agcagcagac	С		4	3	3	1					

Key for efficient pattern matching: how to find the corresponding chars in the first column efficiently, in terms of both time and space.

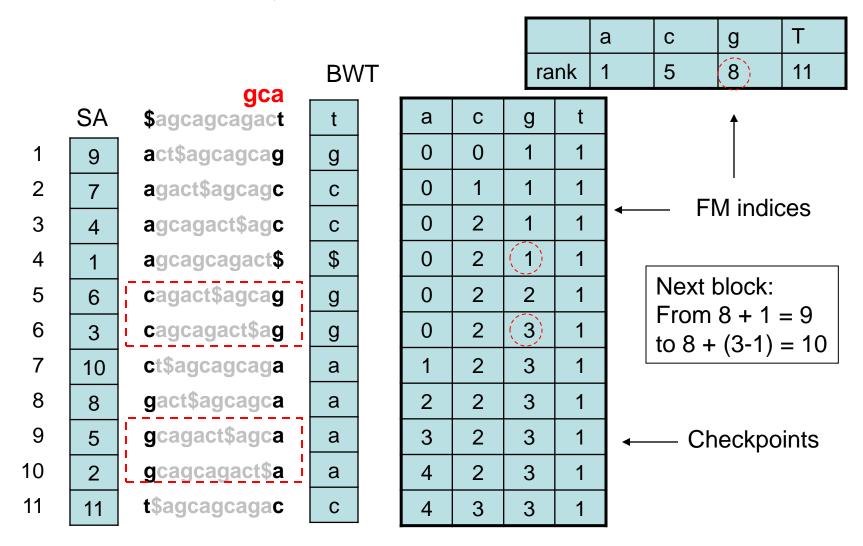
TOTAL



Key for efficient pattern matching: how to find the corresponding chars in the first column efficiently, in terms of both time and space.



Key for efficient pattern matching: how to find the corresponding chars in the first column efficiently, in terms of both time and space.



FM Index: small memory footprint

Components of the FM Index:

First column (F): $\sim |\Sigma|$ integers

Last column (L): m characters

SA sample: $m \cdot a$ integers, where a is fraction of rows kept

Checkpoints: $m \times |\Sigma| \cdot b$ integers, where b is fraction of

rows checkpointed

Example: DNA alphabet (2 bits per nucleotide), T = human genome, a = 1/32, b = 1/128

First column (F): 16 bytes

Last column (L): 2 bits * 3 billion chars = 750 MB

SA sample: 3 billion chars * 4 bytes/char / $32 = \sim 400 \text{ MB}$

Checkpoints: $3 \text{ billion * 4 bytes/char } / 128 = \sim 100 \text{ MB}$

Total < 1.5 GB

End of Ch32