Bit-Parallel Algorithms for Exact Search of Extended Patterns

Algorithms for Sequence Analysis

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Review and Today's Lecture

Reminder

- Horspool's Algorithm:
  $O(mn)$ time worst-case, $O(n/m)$ best-case with long shifts
- Shift-And Algorithm:
  $O(mn/w)$ time, **bit-parallel**, w is register width (64 bits)

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This lecture: More on bit-parallel algorithms

1. How to get **longer shifts** than Horspool's algorithm?
   $\rightarrow$ **BNDM algorithm** (backward non-deterministic DAWG matching)
2. Bit-parallel algorithms for more **general patterns**

Backward Non-Deterministic DAWG Matching

Reminder: Horspool's Algorithm

Horspool shift function

Text:	`?????A?????`	`?????B?????`	`?????C??????`
Pattern:	`BAAAAB`	`BAAAAB`	`BAAAAB`

Approach

- Compare characters **from right to left** in current window
- Shift window based on **last character only**

Weak points

Small alphabets lead to short shifts (especially bad for long patterns).

Substring-based Shifts

Ideas

- Read from right to left (like Horspool)
- **Read on** after mismatch to achieve longer shifts
- When current **substring** of window is not a **substring** of pattern, window can be shifted beyond that **substring**.
- Tracking **window suffixes** that are **pattern prefixes** further increases shifts.

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Requirements for supported queries

- Add characters from right to left
- Is window read so far a **substring** of the pattern?
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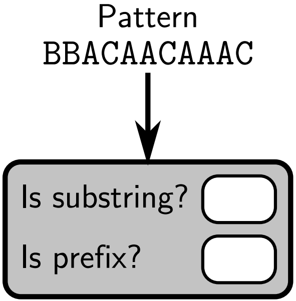

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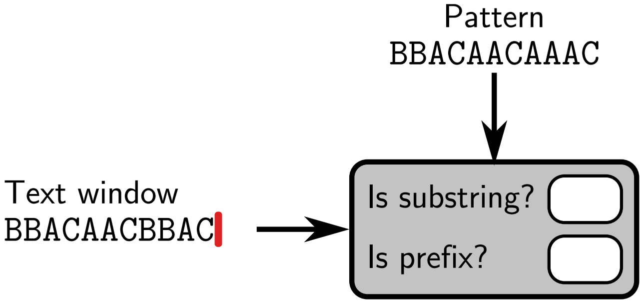

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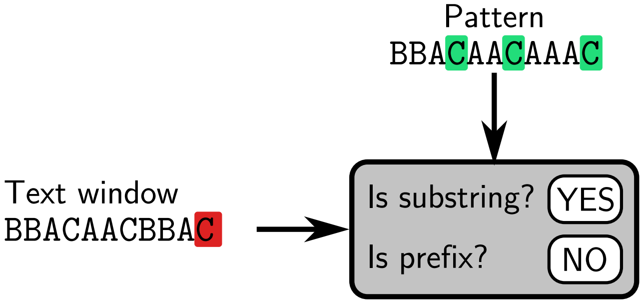

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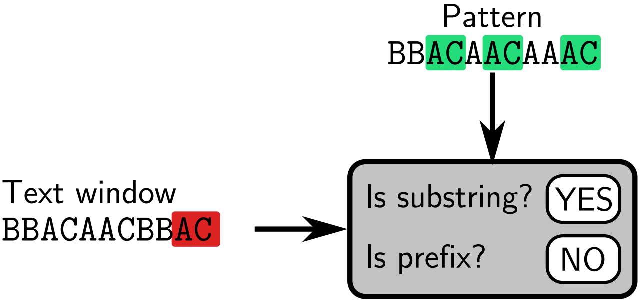

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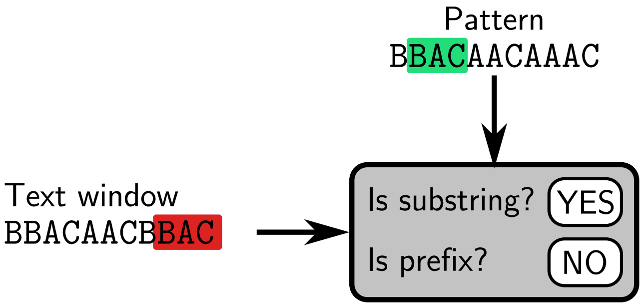

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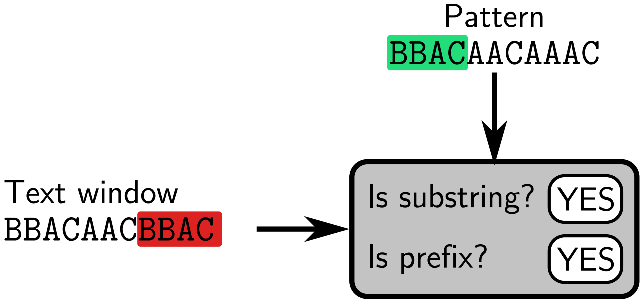

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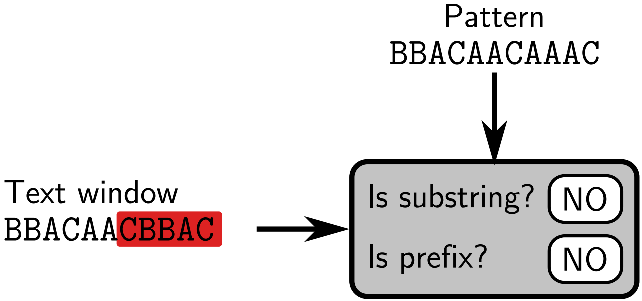
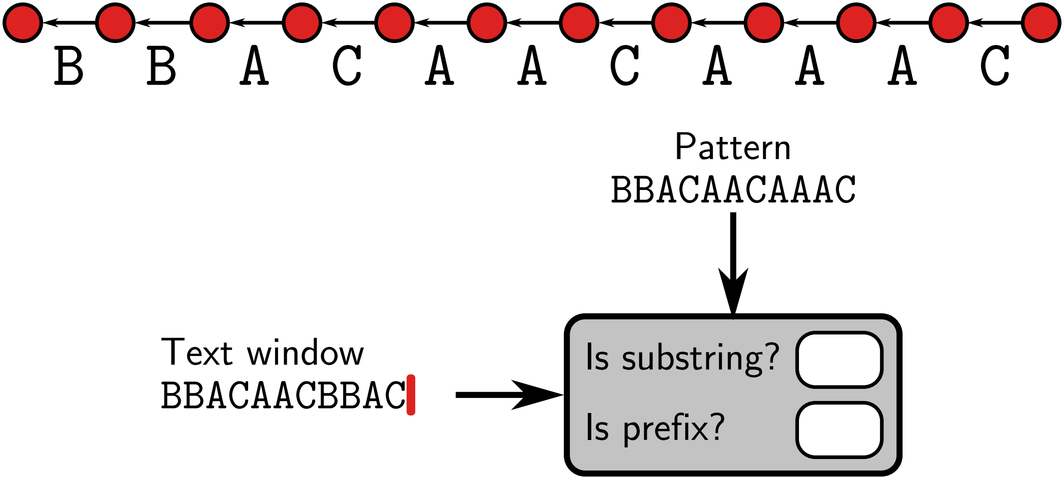


Solution: Non-deterministic suffix automaton



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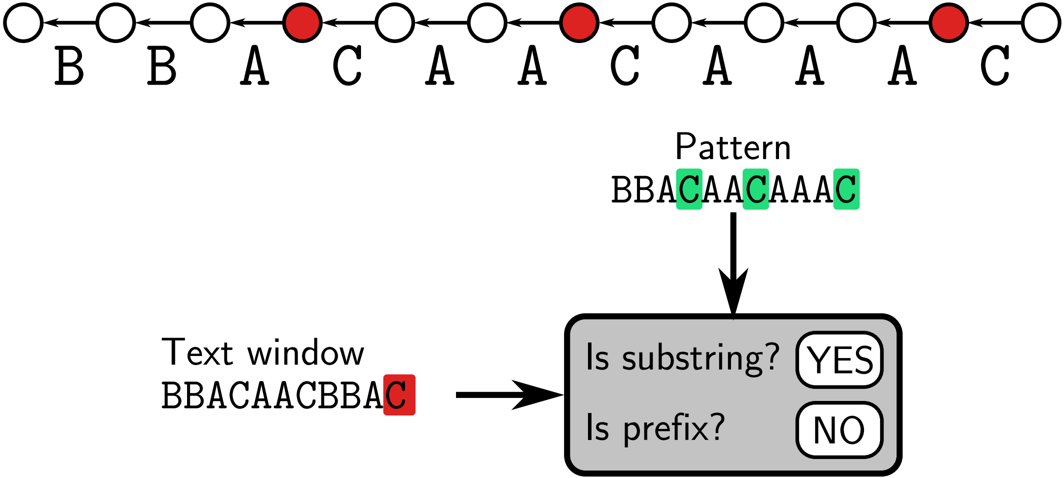

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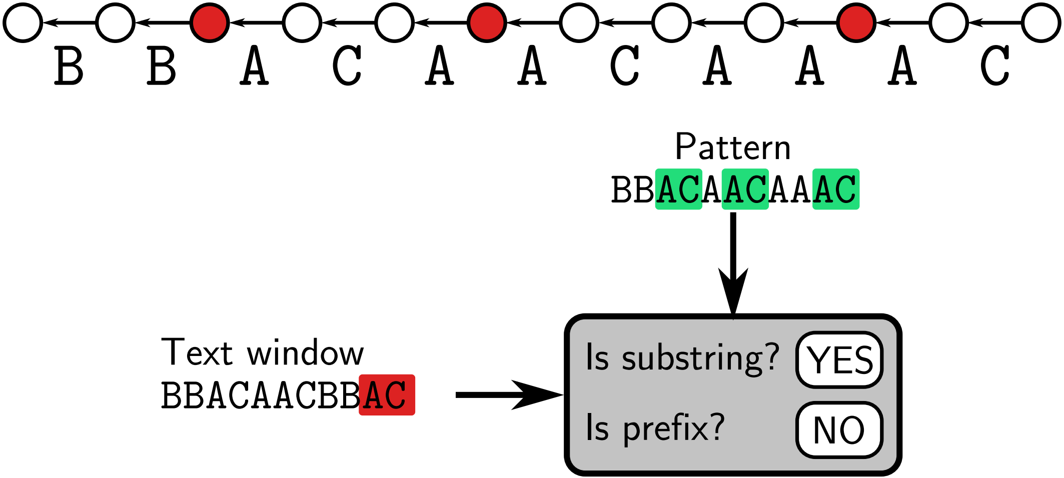

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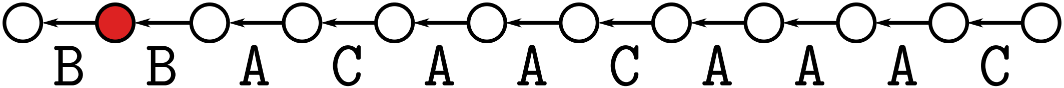

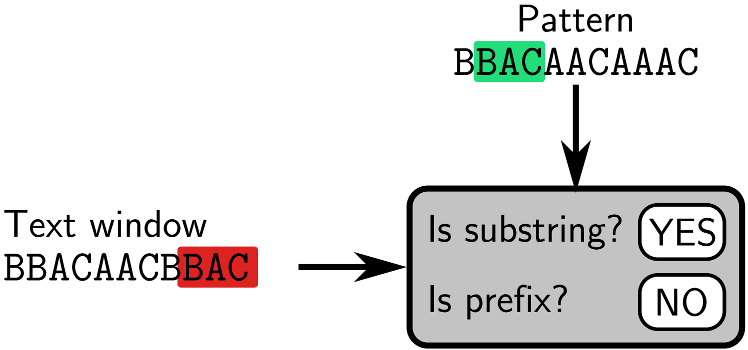

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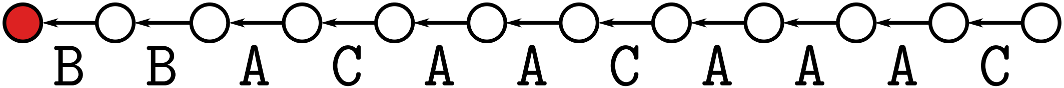

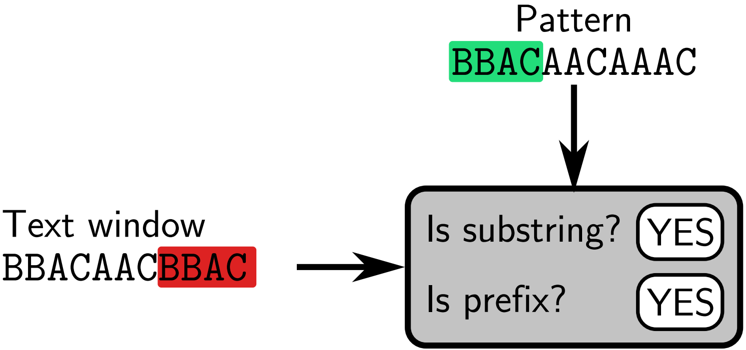

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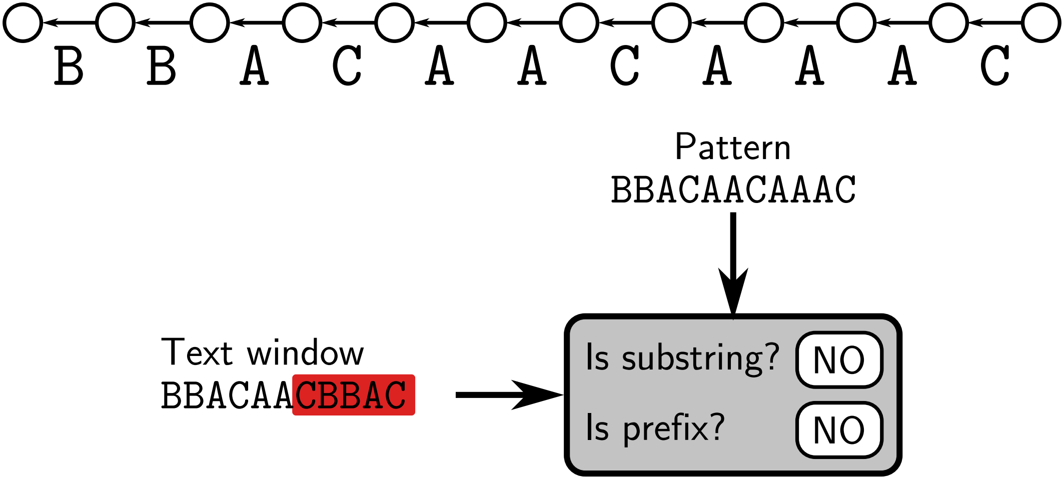
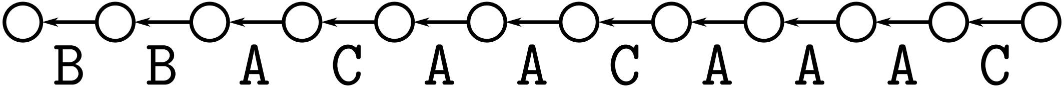


Non-Deterministic Suffix Automaton



Construction

- Construct Pattern Search NFA of **reverse pattern**.
- Do not use a self-loop inside the first (rightmost) state.
- **All** states are start states.

Usage

- Use Shift-And approach to maintain set of active states
- **Any** state is active $\Leftrightarrow$ substring occurs in pattern
- **Accept** state is active $\Leftrightarrow$ found prefix
- **Accept** state is active **and** $|P|$ characters processed $\Leftrightarrow$ found match

BNDM Algorithm

BNDM Algorithm Outline

For **each window**:

1. **Initialize** suffix automaton (all states active)
2. Read window from **right to left** until no states active or full window read.
3. Keep track of **longest window suffix** that is a **pattern prefix**.
4. **Shift** window to **align** this suffix with pattern prefix

BNDM Algorithm: Code

```
def BNDM(P, T):
    masks, accept_state = compute_masks(P[::-1])
    n, m, pos = len(T), len(P), len(P)
    while pos <= n:
        j, lastsuffix, A = 1, 0, (1 << m) - 1
        while A != 0:
            A &= masks[T[pos-j]]         # update A
            if A & accept_state != 0:    # accept state?
                if j == m:   # full pattern found?
                    yield (pos - m, pos)
                    break
                else:          # no, found proper prefix
                    lastsuffix = j   # store suffix
            j += 1;  A = A << 1 # go to next window character
        pos += m - lastsuffix    # shift window
```

Deterministic Counterpart: BDM

Names

- **BDM**: Backward DAWG Matching
- **BNDM**: Backward Non-deterministic DAWG Matching
- **DAWG**: Directed Acyclic Word Graph

BDM (Backward DAWG Matching) Algorithm

- As before, we could transform the NFA into a DFA
  $\rightarrow$ **deterministic suffix automaton** (a DAWG)
- Use the subset construction (can be inefficient),
  use a suffix tree (later),
  or really just used BNDM instead of BDM (if $|P| \leq 64$)

Bit-Parallel Algorithms for Extended Patterns

Overview

So far, patterns were simple strings, $P \in \Sigma^*$.
For several applications (e.g., transcription factor binding sites on DNA), it is necessary to consider patterns that allow

- different characters (some subset of Σ) at some positions,
- variable-length runs of arbitrary characters,
- optional characters at some positions.

All of these patterns are subsets of **regular expressions**, which can be searched for by DFAs.

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Why talk about it?

Specialized **bit-parallel** implementations for each pattern class are more efficient.
All of the above patterns can be recognized by variations of the **Shift-And** algorithm.

Generalized Strings

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  It can be written as a single generalized string: $\{\,\mathrm{M}\,\}\{\,\mathrm{a,e}\,\}\{\,\mathrm{i,y}\,\}\{\,\mathrm{e}\,\}\{\,\mathrm{r}\,\}$.
  Shorthand: M[ae][iy]er

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  Larger sets are represented by square brackets: [ae] for { a,e }.
  We write # for $\Sigma \in 2^\Sigma$ ("any charachter").
- In DNA sequences, the IUPAC code specifies a one-letter code for each subset:
  size 1: `ACGT`;   size 2: `SWRYKM`;   size 3: `BDHV`;   size 4: `N`.

The Shift-And Algorithm for Generalized Strings

- Recall the Shift-And algorithm with active state bits D:
  $D \leftarrow ((D \ll 1) \mid 1)\ \&\ \mathrm{mask}(c)$
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  It is no problem that more than one bit is set at some positions.
- **Example:** $P = \texttt{abba\#b}$ over $\Sigma = \{\texttt{a}, \texttt{b}\}$.

	`b#abba` (reversed because of bit numbers)
$\mathit{mask}[\texttt{a}]$	`011001`
$\mathit{mask}[\texttt{b}]$	`110110`

Bounded-length Runs of Arbitrary Characters

- A **run of arbitrary characters** is a sequence of Σs (written as #s) in a generalized string.
- We allow **variable run lengths**, but with fixed **lower and upper bounds**.
- **Notation:** $\#(L, U)$ with lower bound L and upper bound U
- **Example:** $P = \texttt{bba\#(1,3)a}$:
  After `bba`, we have one to three arbitrary characters, followed by `a`.

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- **Example:** $P = \texttt{bba\#(1,3)a}$:
  After bba, we have one to three arbitrary characters, followed by a.
- Three restrictions:
  1. An element $\#(L, U)$ does not appear first or last in the pattern.
     (We could remove them without substantially changing the pattern.)
  2. No two such elements appear next to each other.
     (No problem, just add them: $\#(L, U)\#(L', U') \mathrel{\widehat{=}} \#(L + L', U + U')$.)
  3. We require $1 \leq L \leq U$.
     (Allowing $L = 0$ is technically more challenging.)

An NFA for Bounded-length Runs of Arbitrary Characters

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- The ϵ-transitions allow us to skip the optional characters.
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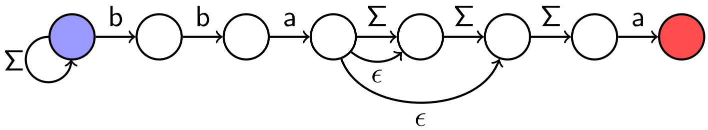
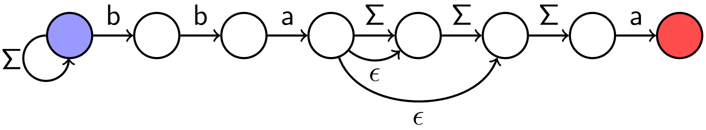
Example: $P =$ `bba#(1,3)a`:



Bit-parallel Implementation



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- Masks are constructed as before (for #: 1-bits for each character).

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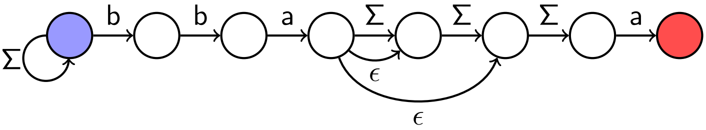

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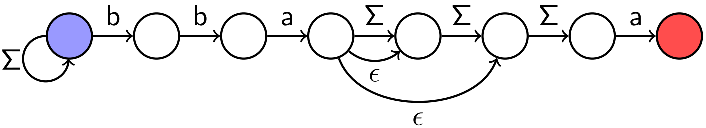
- **Example:** $P =$ `bba#(1,3)a` with $\Sigma = \{a, b, c\}$:

	a###abb
mask[a]	1111100
mask[b]	0111011
mask[c]	0111000

Implementation of ϵ-Transitions



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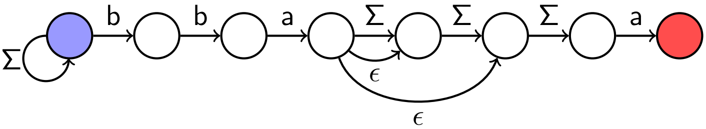

- ϵ-transitions are instantaneous:
  Whenever a state with outgoing ϵ-transitions becomes active (1-bit), this is immediately propagated to the targets of the outgoing ϵ-edges; these are by construction adjacent to the source state.
- The actual propagation of 1-bits will be achieved by subtraction (next slide).
- We use two additional bit masks:
  - Bit mask I marks states with outgoing ϵ-transitions.
  - Bit mask F marks the state after the target of the last ϵ-transition of each run.

	`a###abb`
F	`0100000`
I	`0000100`

Propagation of Ones

- Let A be the bit mask of active states. Then $A \,\&\, I$ selects active I-states.
- Subtraction $F - (A \,\&\, I)$ propagates 1-bits, zeroes F-bits.

$$
\begin{array}{lr}
F & 0100000 \\
A \,\&\, I & 0000100 \\
\hline
- & 0011100
\end{array}
$$

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- **Problem:** Inactive I-states keep corresponding F-bit set:

$$\begin{array}{ll} F & 010000100000 \\ A \mathbin{\&} I & 000000000100 \\ \hline - & 010000011100 \end{array}$$

Propagation of Ones (Continued)

- **Problem:** Inactive I-states keep corresponding F-bit set.
- **Solution:** Zero out F-bits by a bitwise `and` with the negation of F:

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$\sim F$	101111011111
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$\sim F$	101111011111
$(F - (A \,\&\, I)) \,\&\, \sim F$	000000011100

- The resulting modified Shift-And update is thus:
  1. Apply standard Shift-And update:
     `A = ((A << 1) | 1) & mask[c]`
  2. Propagate active I-states along ϵ-transitions:
     `A = A | ((F - (A & I)) & ~F)`

Patterns with Optional Characters

- Another modification of the Shift-And algorithm allows optional characters.
- **Notation:** Write `?` after the optional character.
- **Example:** The set {color, colour} becomes $P = \texttt{colou?r}$.
- Consecutive optional characters (“blocks”) are allowed.

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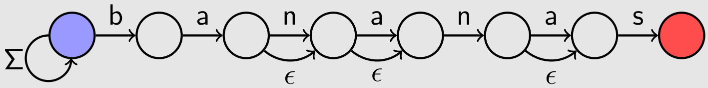
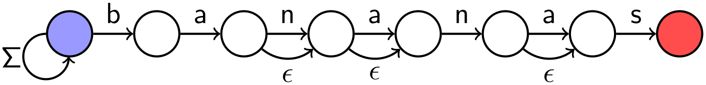
Larger example: $P =$ `ban?a?na?s` and $T =$ `banabanns`



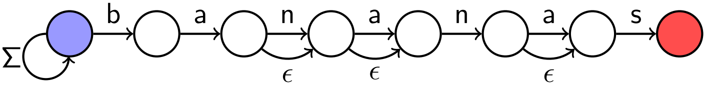
Bit-Parallel Implementation of Optional Characters



I :	0	1	0	0	1	0	0
F :	0	0	0	1	0	1	0
O :	0	0	1	1	0	1	0

- Three bit masks:
  I: block start; O: targets of ϵ-transitions; F: block end
- Note: actual bit patterns are reversed (bit numbering vs. state numbering).

Bit-Parallel Implementation of Optional Characters



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- Activity of any state within a block must be propagated to the block's end: Propagate the lowest active bit within a block up to the F-bit.
- Consider how 1-bit propagation via subtraction works:

```
  1101010000          1101011000
-          1        -        100
------------        ------------
  1101001111          1101010100
```

- Bits to the left (green) and to the right (black) are unchanged; only bits between the rightmost ones in the current block change (red).

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```

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- We develop the machinery by example:

```
A   .0010100.                         A  .0010100.
I   .0000001.                       A|F  .1010100.
O   .1111110.                   (A|F)-I  .1010011.
F   .1000000.           ((A|F)-I)=(A|F)  .1111000.
|                     O&((A|F)-I)=(A|F)  .1111000.
>>  .1111100.      A|(O&((A|F)-I)=(A|F))  .1111100.
```

Bit-Parallel Implementation of Optional Characters (Conclusion)

- **Note:** Bitwise equality $X = Y$ can be implemented as $\sim(X \oplus Y)$.
- Full implementation:
  1. Create masks for all characters;
     treat optional characters as regular characters.
  2. Standard Shift-And update of active states A:
     `A = ((A << 1) | 1) & mask[c]`
  3. Propagate active states over optional characters:
     `AF = A | F`
     `A = A | (O & (~(AF - I) ^ AF))`
     (Here, ^ denotes the xor-operation.)

Summary

Topic

Bit-parallel methods for exact pattern matching of single patterns without text indexing

Properties of bit-parallel algorithms

- Typically only applicable if an "almost linear" NFA recognizes the pattern, and if this NFA has at most 64 (register width) states
- Shift-And approach is simple and very flexible, extends to general patterns; running time is always $O(n)$ for constant $|P| < 64$.
- BNDM approach is also simple and flexible; may pathologically use $O(mn)$ time even for constant $m = |P| < 64$, but has best-case running time of $O(m + n/m)$.

Possible exam questions

- Explain the idea of bit-parallel simulation of NFAs.
- Explain the suffix automaton and the BNDM algorithm.
- What are the advantages of BNDM over Horspool's algorithm?
- What are the advantages of BNDM over the Shift-And algorithm?
- What is a generalized string?
- How does the Shift-And algorithm change when you allow generalized strings?
- Why would you want to use the Shift-And algorithm for runs with bounded length, when the algorithms for optional characters is more general ($\#(3,5) = \#?\#?\#\#\#$)?
- How do you implement bit-parallel propagation of an active state?

Conclusion

Topic

Exact pattern matching of single patterns without text indexing

Strengths of different algorithms

- **Shift-And:** simple, applicable if $|P| \leq 64$
- **B(N)DM:** for $|P| < 64$; best case of $O(m + n/m)$;
  long shifts even for small alphabet + long pattern
- **Horspool:** best case of $O(m + n/m)$ for large alphabet + long pattern
- **Knuth-Morris-Pratt (KMP):** best worst-case time of $O(m + n)$

- Automata theory was very useful.
- Next topic: index structures (i.e. preprocessing the text)