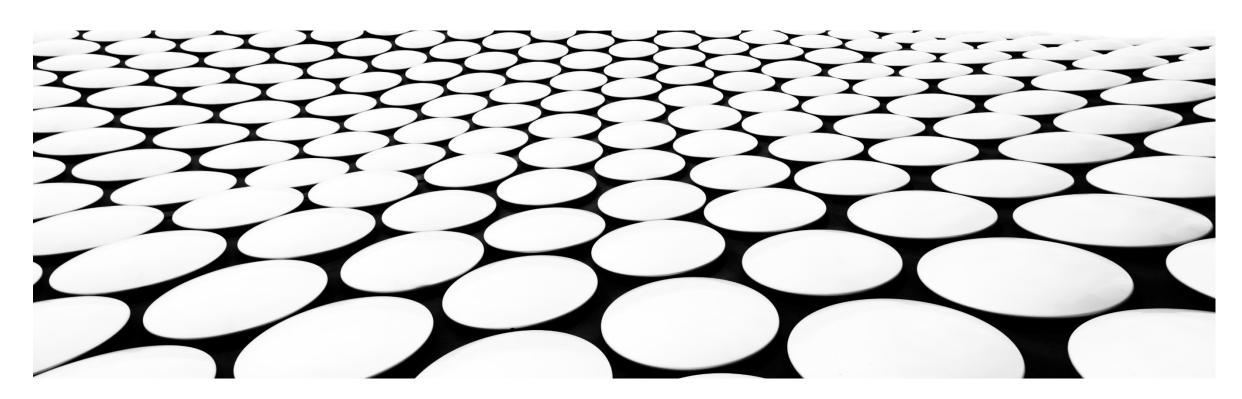
BIOINFORMATICS(BIOCOMPUTING)

(4)

BOYER-MOORE

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String Definitions

A *string* S is a finite ordered list of characters.

Characters are drawn from an alphabet Σ .

Nucleic acid alphabet: { A, C, G, T }
Amino acid alphabet: { A, R, N, D, C, E, Q, G, H, I, L, K, M, F, P, S, T, W, Y, V }

Length of S, |S|, is the number of characters in S

 ϵ is the empty string. $|\epsilon| = 0$

String Definitions

- For strings S and T over Σ, their concatenation consists of the characters of S followed by the characters of T, denoted ST
- S is a substring of T if there exist (possibly empty) strings u and v such that
 T = uSv
- S is a prefix of T if there exists a string u such that T = Su. If neither S nor u are ϵ , S is a proper prefix of T.
- Definitions of suffix and proper suffix are similar.

String Definitions

• We defined substring. Subsequence is similar except the characters need not be consecutive.

• "cat" is a substring and a subsequence of "concatenate"

 "cant" is a subsequence of "concatenate", but not a substring

Exact matching

- Looking for places where a *pattern P* occurs as a substring of a *text T*. Each such place is an *occurrence* or *match*.
- An *alignment* is a way of putting *P's* characters opposite *T's* characters. It may or may not correspond to an occurrence.

At what offsets does *pattern P* occur within *text T*?

P: word

T: There would have been a time for such a word

Answer: offset 40

Exact Matching

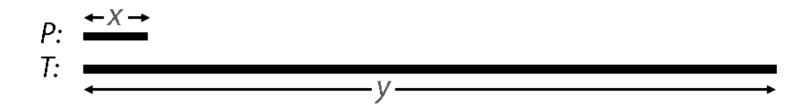
At what offsets does *pattern P* occur within *text T*?

```
>>> t = 'There would have been a time for such a word'
>>> t.find('word')
40
```

Exact matching: naïve algorithm

Let
$$x = |P|, y = |T|$$

How many alignments are possible given x and y?



$$y - x + 1$$

Exact matching: naïve algorithm

Let
$$x = |P|, y = |T|$$

What's the greatest # character comparisons possible?

P: aaaa

$$x(y - x + 1)$$

Exact matching: naïve algorithm

Let
$$x = |P|, y = |T|$$

What's the least # character comparisons possible?

P: abbb

$$y - x + 1$$

Can we improve on the naïve algorithm?

udoesn't occur in P, so skip next two alignments

Boyer-Moore

Learn from character comparisons to skip pointless alignments

1. When we hit a mismatch, move *P* along until the mismatch becomes a match

"Bad character rule"

2. When we move *P*along, make sure characters that matched in the last alignment also match in the next alignment

"Good suffix rule"

3. Try alignments in one direction, but do character comparisons in *opposite* direction

For longer skips

P: word

T: There would have been a time for such a word



Boyer-Moore: Bad character rule

Upon mismatch, skip alignments until:

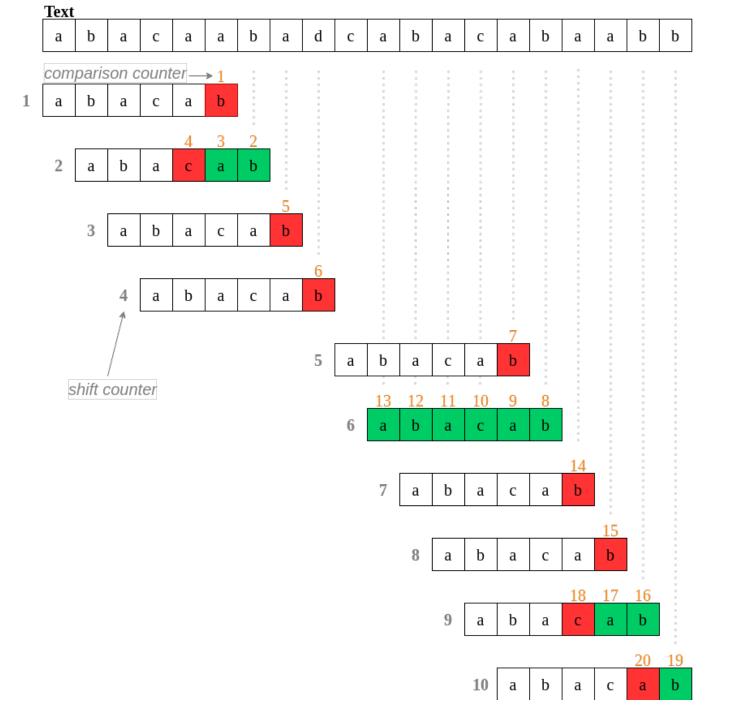
- (a) mismatch becomes a match, or
- (b) Pmoves past mismatched character.
- (c) If there was no mismatch, don't skip

```
T: GCTTCTGCTACCTTTTGCGCGCGCGCGA
Step 1:
      A CCTTTTGC
                                           Case (a)
      T: GCTTCTGCT(A)CCTTTTGCGCGCGCGCGA
Step 2:
                                           Case (b)
      T: GCTTCTGCTACCTTTTGCGCGCGCGCGA
Step 3:
                                           Case (c)
      P:
      T: GCTTCTGCTACCTTTTGCGCGCGCGCGAA
Step 4:
                      CCTTTTGC
 (etc)
```

Boyer-Moore: Bad character rule

Up to step 3, we skipped 8 alignments

5 characters in Twere never looked at



Boyer-Moore: Good suffix rule

Let t = substring matched by inner loop; skip until (a) there are no mismatches between P and t or (b) P moves past t

```
Step 1: T: CGTGCCTACTTACTTACTTACGCGAA

P: CTTACTTAC

Step 2: T: CGTGCCTACTTACTTACTTACGCGAA

P: CTTACTTAC

Step 3: T: CGTGCCTACTTACTTACTTACGCGAA

CTTACTTAC
```

Boyer-Moore: Good suffix rule

Let t = substring matched by inner loop; skip until (a) there are no mismatches between P and t or (b) P moves past t

```
Step 1: T: CGTGCCTACTTACTTACTTACGCGAA

P: CTTACTTAC

toccurs in its entirety to the left within P

Step 2: T: CGTGCCTACTTACTTACTTACGCGAA

P: CTTACTTAC

prefix of Pmatches a suffix of t

Step 3: T: CGTGCCTACTTACTTACTTACGCGAA

CTTACTTAC
```

Case (a) has two subcases according to whether toccurs in its entirety to the left within P (as in step 1), or a prefix of P matches a suffix of t (as in step 2)

Boyer-Moore: Putting it together

How to *combine* bad character and good suffix rules?

```
T: GTTATAGCTGATQGCGGCGTAGCGGCGAA
P:
```

bad char says skip 2, good suffix says skip 7 Take

the maximum! (7)

Boyer-Moore: Putting it together

Use bad character or good suffix rule, whichever skips more

```
T: GTTATAGC TGATCGCGGCGTAGCGGCGAA
Step 1:
       P: G(T)A G C G G C_G
                                              bc:6, gs:0 bad character
      T: GTTATAGCTGATQGCGGCGTAGCGGCGAA
Step 2:
                    G T A G C G G C G
                                              bc: 0, qs: 2 good suffix
       T: GTTATAGCTGATCGCGGCGTAGCGGCGAA

P: bc:2, gs:7
Step 3:
                                              bc: 2, qs: 7 good suffix
           GTTATAGCTGATCGCGGCGTAGCGGCGAA
Step 4:
                                      GTAGCGGCG
```

11 characters of *T* we ignored

Step 1: T: GTTATAGCTGATCGCGGCGTAGCGGCGAA
P: GTAGCGGCG

Step 2: T: GTTATAGCTGATCGCGGCGTAGCGGCGAA
GTAGCGGCG

Step 3: T: GTTATAGCTGATCGCGGCGTAGCGGCGAA
P: GTAGCGGCG

Step 4: T: GTTATAGCTGATCGCGGCGTAGCGGCGAA

GTAGCGGCG

GTAGCGGCGAA

Skipped 15 alignments

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and P = TCGC:

| | | Р | | | | | | | | |
|---|---|---|---|---|---|--|--|--|--|--|
| | | Т | С | G | С | | | | | |
| | Α | | | | | | | | | |
| Σ | С | | ı | | - | | | | | |
| | G | | | ı | | | | | | |
| | Т | - | | | | | | | | |

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and P = TCGC:

| | | | | P | |
|---|---|---|---|---|---|
| | | Т | С | G | С |
| | Α | 0 | 1 | 2 | 3 |
| Σ | С | 0 | ı | 0 | - |
| | G | 0 | 1 | ı | 0 |
| | | ı | 0 | 1 | 2 |

T: A ATC A A T A G C Skip: 1 alignments (2 shifts)

This can be constructed efficiently.

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and P = TCGC:

| | | | ı | P | | | |
|---|---|---|---|---|---|---|--------------------|
| | | Т | С | G | | T: A ATC A A T C G C | |
| | A | 0 | 1 | 2 | 3 | P: TCGC | |
| Σ | С | 0 | - | 0 | ı | <i>Τ</i> · Δ Δ Τ C Δ <mark>Δ</mark> Τ C G C | Skip: 3 alignments |
| | G | 0 | 1 | ı | 0 | T: AATCAATCGC P: TCGC | (4 shifts) |
| | Т | - | 0 | 1 | 2 | | |

This can be constructed efficiently.

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and P = TCGC:

| | | | 1 | P | | |
|---|---|---|---|---|---|------------------------------|
| | | Т | С | G | С | T: A ATC A A T A G C P: TCGC |
| | Α | 0 | 1 | 2 | 3 | T: AATCAATAGC |
| Σ | С | 0 | - | 0 | ı | <i>P:</i> T C G C |
| | G | 0 | 1 | ı | 0 | T: AATCAATCGC |
| | Т | - | 0 | 1 | 2 | P: TCGC |

This can be constructed efficiently.

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P* = GTAGCGGCG

| | | | P | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|--|--|--|--|
| | | G | Т | Α | G | С | G | G | С | G | | | | |
| | Α | | | | | | | | | | | | | |
| Σ | С | | | | | | | | | | | | | |
| | G | | | | | | | | | | | | | |
| | Т | | | | | | | | | | | | | |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P* = GTAGCGGCG

| | | | | | | <u>P</u> | | | | _ |
|---|---|---|---|---|---|----------|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | | | ı | | | | | | |
| Σ | С | | | | | ı | | | 1 | |
| | G | ı | | | ı | | ı | ı | | I |
| | Т | | _ | | | | | | | |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P*= GTAGCGGCG

| | | | | | | P | | | | _ |
|---|---|---|---|---|---|---|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | ı |
| | Т | 0 | - | 0 | 1 | 2 | 3 | 4 | 5 | 6 |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P* = GTAGCGGCG

| | | | | | | P | _ | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | ı |
| | Т | 0 | - | 0 | 1 | 2 | 3 | 4 | 5 | 6 |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and P = GTAGCGGCG

| | | | | | | P | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | - |
| | Т | 0 | - | 0 | 1 | 2 | 3 | 4 | 5 | 6 |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P* = GTAGCGGCG

| | | | | | | P | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | ı |
| | Т | 0 | _ | 0 | 1 | 2 | 3 | 4 | 5 | 6 |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P* = GTAGCGGCG

| | | | | | | P | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | ı |
| | Т | 0 | 1 | 0 | 1 | 2 | 3 | 4 | 5 | 6 |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P* = GTAGCGGCG

| | | | | | | <u>P</u> | | | | |
|---|---|---|---|---|---|----------|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | ı |
| | Т | 0 | - | 0 | 1 | 2 | 3 | 4 | 5 | 6 |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and *P* = GTAGCGGCG

| | | P | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | G | Т | Α | G | С | G | G | С | G |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | ı |
| | Т | 0 | - | 0 | 1 | 2 | 3 | 4 | 5 | 6 |

P: GTAGCGGCG

Pre-calculate skips for all possible mismatch scenarios! For bad character rule and P = GTAGCGGCG

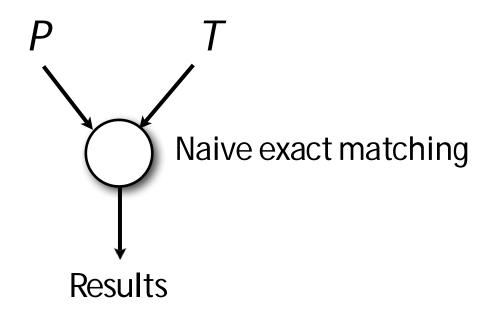
| | | <u> </u> | | | | | | | | | |
|---|---|----------|---|---|---|---|---|---|---|---|--|
| | | G | Т | Α | G | С | G | G | С | G | |
| | Α | 0 | 1 | ı | 0 | 1 | 2 | 3 | 4 | 5 | |
| Σ | С | 0 | 1 | 2 | 3 | ı | 0 | 1 | ı | 0 | |
| | G | ı | 0 | 1 | ı | 0 | ı | ı | 0 | ı | |
| | Т | 0 | ı | 0 | 1 | 2 | 3 | 4 | 5 | 6 | |

P: GTAGCGGCG

As with bad character rule, good suffix rule skips can be precalculated efficiently.

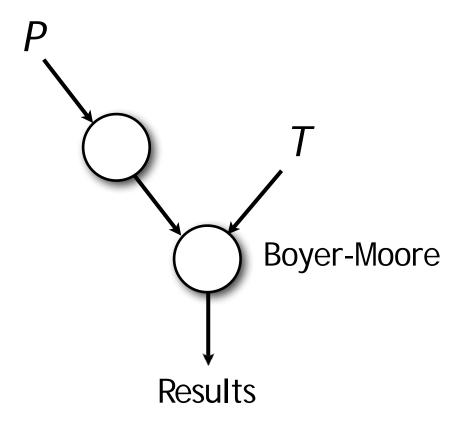
For both tables, the calculations only consider *P*. No knowledge of *T* is required.

Preprocessing: Naive algorithm



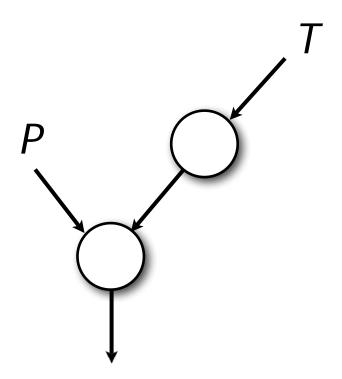
Preprocessing: Boyer-Moore

Preprocess P: Make lookup tables for bad character & good suffix rules



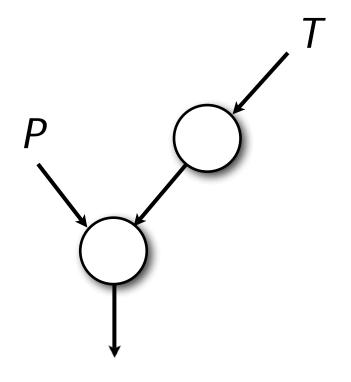
Preprocessing

Preprocess T (offline): Genome or sequence that does not have frequent changes.



Preprocessing

Algorithm that preprocesses *T* is *offline*. Otherwise, algorithm is *online*.



Online or offline?

- Naïve algorithm
- Boyer-Moore
- Web search engine
- Read alignment









You have a pattern P and you expect to receive several texts T1, T2, T3, ..., and you would like to match P against each text as it arrives. It is better to use an algorithm that:

Preprocesses T Preprocesses P Preprocesses neither P nor T

An online algorithm does not:

Preprocess P Preprocess at all