# Exact pattern matching & string search



# Why Exact Matching?

As *loose* motivation, consider the problem of mapping a read r to the genome G.

In reality, we would not use exact matching for this; why?

However, exact matching is useful here:

 Find all places where a substring of the query matches the reference exactly (seeds)

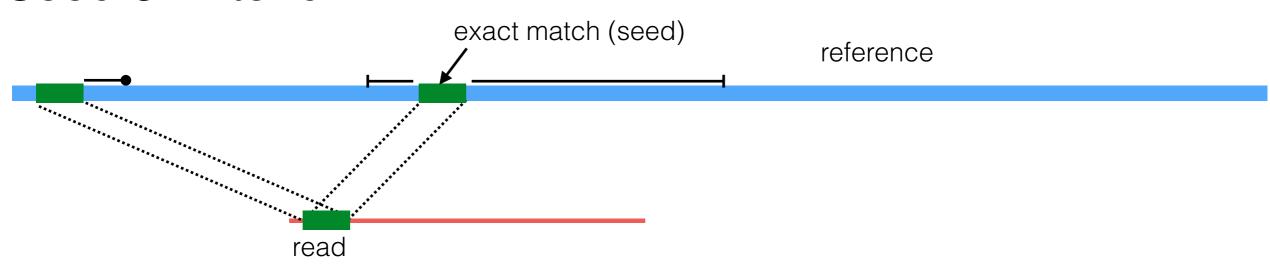
Requires efficient exact search

- Filter out regions with insufficient exact matches to warrant further investigation
- Perform a "constrained" alignment that includes these exact matching "seeds"

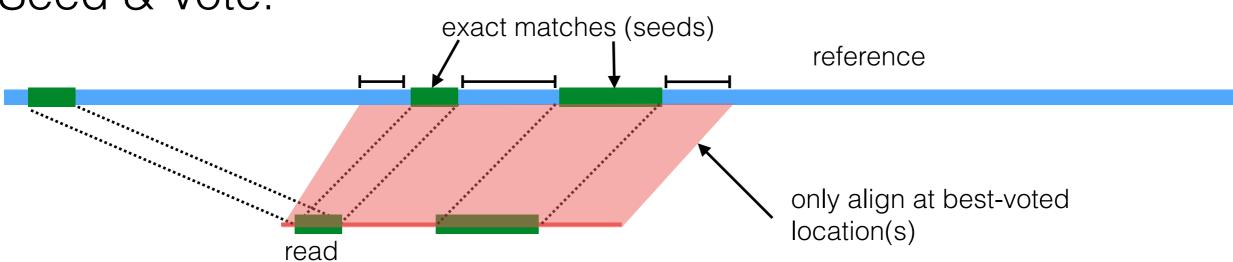
Here is where we use our alignment DPs

# Typical Strategies

#### Seed & Extend:



#### Seed & Vote:



## Exact String Matching Problem

Today, we'll talk about exact matching algorithms that are **quadratic** (no better than alignment!) and **linear**. Then we'll start talking about **much** faster approaches, but they require pre-processing the reference.

# Exact String Matching Problem

**Given:** A string **T** (called the *text*) and a string **P** (called the *pattern*).

Find: All occurrences of P in T.

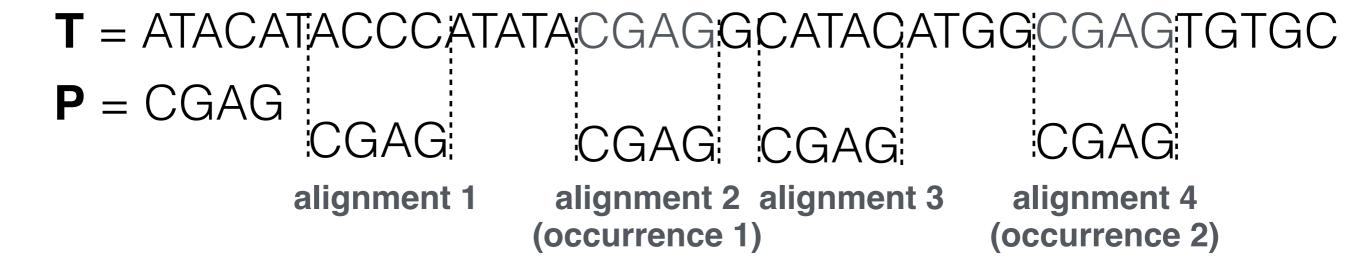
An occurrence of P in T is a substring of T equal to P

T = ATACATACCCATATACGAGGCATACATGGCGAGTGTGC
P = CGAG
CGAG
CGAG

## Occurrences vs. Alignments

An *alignment* of **P** to **T** is a correspondence (not necessarily an occurrence) between a substring of **T** and **P** 

all occurrences are alignments but not all alignments are occurrences



## Occurrences vs. Alignments

How many possible *alignments* of **P** are there in **T**?

```
T = ATACATACCCATATACGAGGCATACATGGCGAGTGTGC
```

```
P = CGAG
CGAG
CGAG
CGAG
CGAG
```

## Occurrences vs. Alignments

How many possible *alignments* of **P** are there in **T**?

```
T = ATACATACCCATATACGAGGCATACATGGCGAGTGTGC
```

```
P = CGAG
CGAG
CGAG
CGAG
```

|T| - |P| + 1

What is the simplest algorithm you can think of to solve the exact string matching problem?

Seriously, I'm not going to change the slide until somebody suggests something really naive!

Naive algorithm 1: Consider all alignments of **P** to **T**, and report each alignment that is an occurrence.

```
def naive(T, P):
    N = len(T)
    M = len(P)
    occs = []
    for i in range(N - M + 1):
        if P == T[i:i+M]:
        occs.append(i)
    return occs
```

```
def naive(T, P):
     N = len(T)
     M = len(P)
     occs = []
     for i in range(N
                          - M + 1):
         if P == T[i:i+M]
                                       O(M) — note,
               occs.append(i)
                                        a "stupid" implementation
     return occs
                                        of this takes M time while a
                                        reasonable version quits at
                                        the first mismatching
                                        character
```

O(N) \* O(M) = O(NM) time

#### Best scenario for naive:

T: GAGAGGAGTTATATATGAATAGAGATAGAGACGAG

P: CGAG

Because every alignment but the last disagrees on the very first character, the inner loop takes O(1) time, except for the single match which takes O(M) time O(N+M)

Worst scenario for naive:

P: CCCCG

P, the inner loop requires M char. compares each time O(NM)

There's a **big** gap between

The best case time for naive O(N+M) and

The worst case time for naive O(NM)

How can we improve the worst case time?

Can we devise a method that is O(N+M) even in the worst case?

T: ATACGGCACATACCATACGAATATACAAA

**Def:** Let  $Z_i$  be the length of the longest substring *starting* at i that matches a prefix of T.

T: ATACGGCACATACCATACGAATATACAAA

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T: ATACGGCACATACCATACGAATATACAAA

Z<sub>T</sub>: -10100001040100501001304010111

**Def:** Let  $Z_i$  be the length of the longest substring *starting* at i that matches a prefix of T.

T: ATACGGCACATACCATACGAATATACAAA

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**Def:** Let  $Z_i$  be the length of the longest substring *starting* at i that matches a prefix of T.

Naïvely, there is an O( ) algorithm to compute the z values

T: ATACGGCACATACCATACGAATATACAAA

Z<sub>T</sub>: -10100001040100501001304010111

**Def:** Let  $Z_i$  be the length of the longest substring *starting* at i that matches a prefix of T.

Naïvely, there is an O(T2) algorithm to compute the z values

Ignore this complexity for a second; how could we use z values to solve exact pattern matching?

P: ACA

T: ATACGGCACATACCATACGAATATACAAA

**Def:** Let  $Z_i$  be the length of the longest substring *starting* at i in T that matches a prefix of P.

Ignore this complexity for a second; how could we use z values to solve exact pattern matching?

P\$T: ACA\$ATACGGCACATACCATACGAATATACAAA

**Def:** Let  $Z_i$  be the length of the longest substring *starting* at i in T that matches a **prefix of P**.

Now, any  $Z_i$  value = |P| designates that an occurrence of P exists at position i in T.

Note:  $\$ \notin \Sigma$  ensures that  $Z_i$  is always  $\le |P|$ 

P\$T: ACA\$ATACGGCACATACCATACGAATATACAAA

Now that the longest possible  $Z_i$  is  $\leq |P|$  then we are back to an O(|T||P|) algorithm ... back to the problem at hand; how do we make this better?

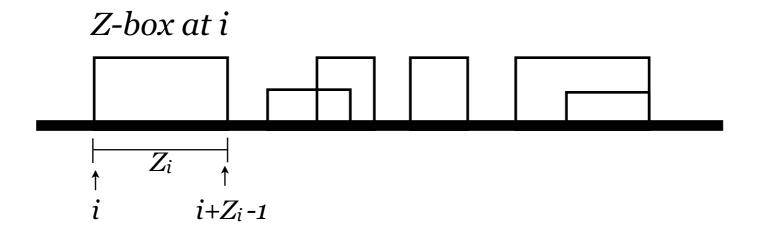
## Z boxes (boxen?)

T: ATACGGCACATACCATACGAATATACAAA

ZT: -10100001040100501001304010111

Imagine a "box" (possibly of length 0) starting at every position. The left-most end of the box is where the match with the prefix begins, and each box extends  $Z_i$  characters to the right (to position  $i + Z_i - 1$ ).

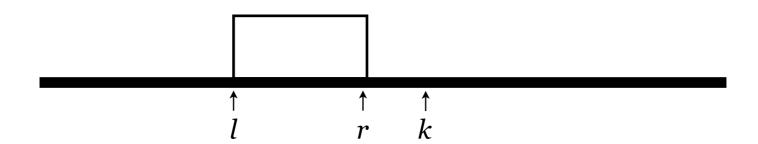
#### **Z** Boxes



**Def.** *Z-box* at *i* is the substring starting at *i* and continuing to  $i+Z_i-1$ . This is the substring that matches the prefix. There is no Z-box at *i* if  $Z_i = 0$ .

- Algorithm for computing  $Z_i$  will iteratively compute  $Z_k$  given:
  - $Z_2...Z_{k-1}$ , and
  - the boundaries l, r of the rightmost Z-box found starting someplace in 2...k-1.
  - you don't need I to understand how the algorithm works, but it is required to efficiently compute the necessary quantities

- Input:  $Z_2...Z_{k-1}$ , and the boundaries I, r of the rightmost Z-box found starting someplace in 2...k-1.
- Output:  $Z_k$ , and updated l, r
- 1. If k > r, explicitly compute  $Z_k$  by comparing with prefix. If  $Z_k > 0$ : l = k and  $r = k + Z_k 1$  (since this is a new farther right Z-box).



The current index is *beyond* the bound of the rightmost z-box.

The structure of the rightmost z-box can not tell us what to expect for Zk

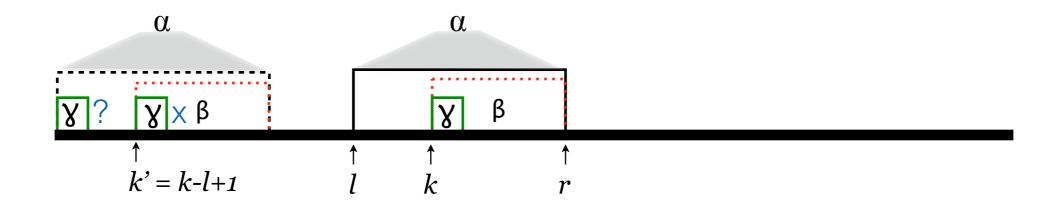
Compute  $Z_k$  by explicit comparison and update I,r if  $Z_k > 0$ 

- Input:  $Z_2...Z_{k-1}$ , and the boundaries I, r of the rightmost Z-box found starting someplace in 2...k-1.
- Output:  $Z_k$ , and updated I, r

If  $k \le r$ , this is the situation:

Case 2a :  $Z_{k'} < |\beta|$ :

 $Z_{k'} < \beta$ : Then the  $\gamma$  that is a prefix of  $\beta$  is also a prefix of  $\alpha$ , **but** the character occurring after the  $\gamma$  starting at k' is *not* the same as the character after the  $\gamma$  starting at the beginning of the string ... why?

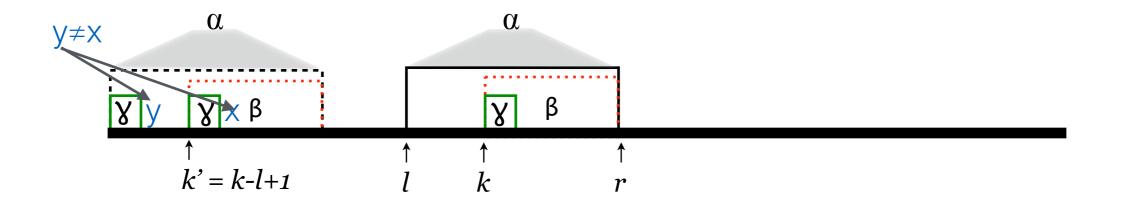


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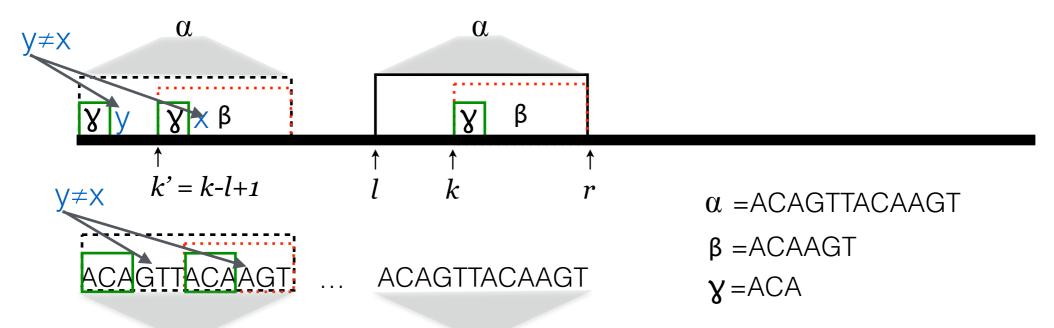


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 $\alpha$ 

e.g.

 $\alpha$ 

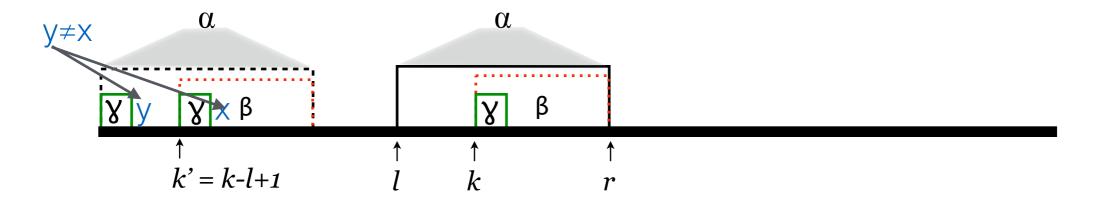
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If x = y, then  $Z_{k'} > |y|$ , because the shared prefix starting at k' and 0 would had to have been longer.



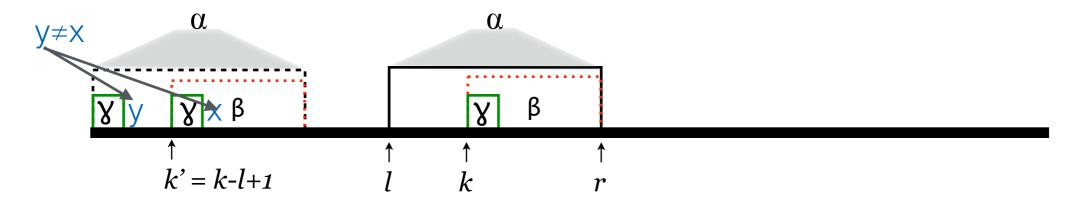
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If x = y, then  $Z_{k'} > |y|$ , because the shared prefix starting at k' and 0 would had to have been longer. But  $\beta = \beta$ , so  $Z_k = Z_{k'}$ 



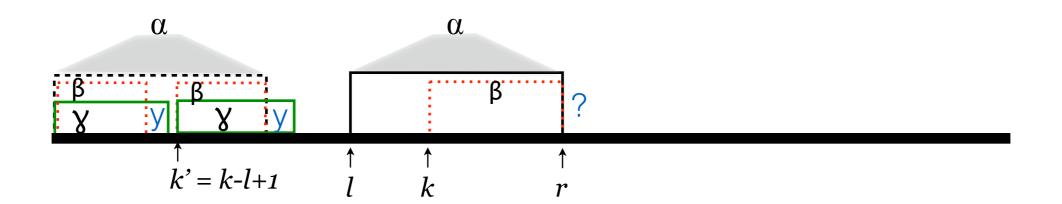
In this case, set  $Z_k = Z_{k'}$  and leave I, r unchanged.

- Input:  $Z_2...Z_{k-1}$ , and the boundaries I, r of the rightmost Z-box found starting someplace in 2...k-1.
- Output:  $Z_k$ , and updated I, r

If  $k \le r$ , this is the situation:

Case 2b :  $Z_{k'} > |\beta|$ :

 $Z_{k'} > |\beta|$ : Then the  $\gamma$  that starts at k' matches the  $\gamma$  that starts at the beginning of T, **but**, it cannot (completely) match the substring starting at k ... why?



- Input:  $Z_2...Z_{k-1}$ , and the boundaries I, r of the rightmost Z-box found starting someplace in 2...k-1.
- Output:  $Z_k$ , and updated I, r

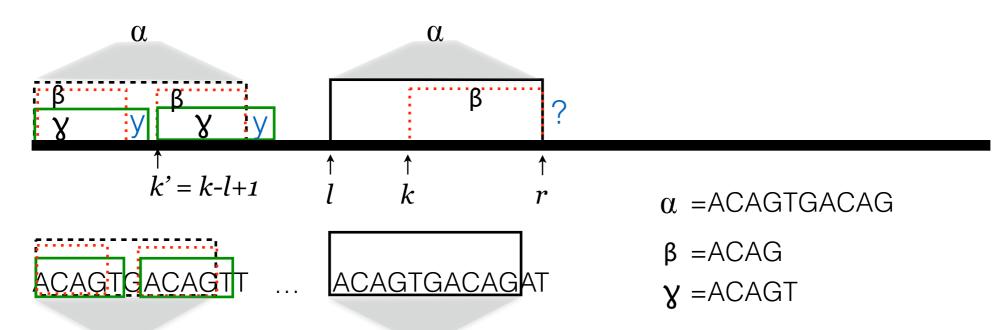
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at k ... why?

Note: Here, we are not necessarily saying that the "Z-box" starting at 0 (ill-defined anyway) is of length  $|\alpha|$ ; Rather  $\alpha$  is defined by  $Z_l$ 



 $\alpha$ 

e.g.

 $\alpha$ 

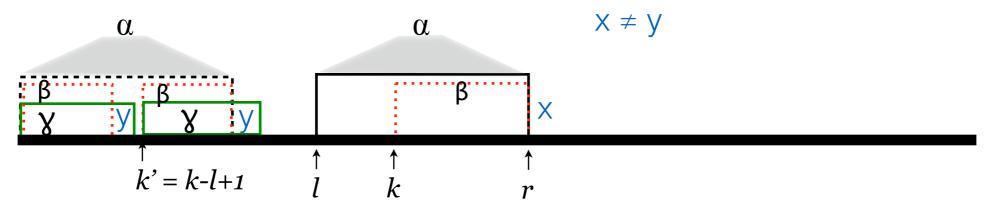
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If it did, then the z-box starting at position I, would be longer (extend past r), contradicting the fact that  $Z_I$  is the *longest* substring starting at I that matches a prefix of T.



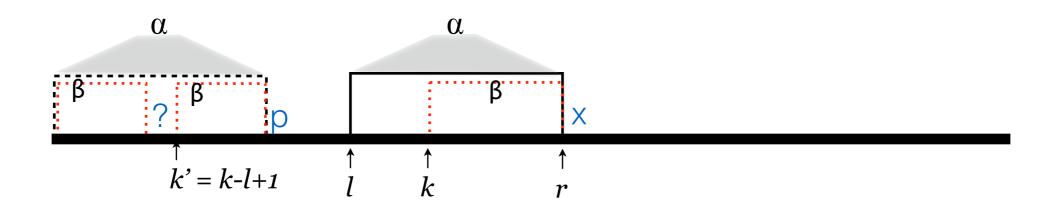
Set  $Z_k = |\beta|$  and leave l, r unchanged.

- Input:  $Z_2...Z_{k-1}$ , and the boundaries I, r of the rightmost Z-box found starting someplace in 2...k-1.
- Output:  $Z_k$ , and updated I, r

If  $k \le r$ , this is the situation:

Case 2c :  $Z_{k'} = |\beta|$ :

 $Z_{k'} = |\beta|$ : Then the character following the z-box of  $Z_{k'}$ , cannot be the same as the character following the length  $\beta$  prefix of the string ... why?



- Input:  $Z_2...Z_{k-1}$ , and the boundaries I, r of the rightmost Z-box found starting someplace in 2...k-1.
- Output:  $Z_k$ , and updated I, r

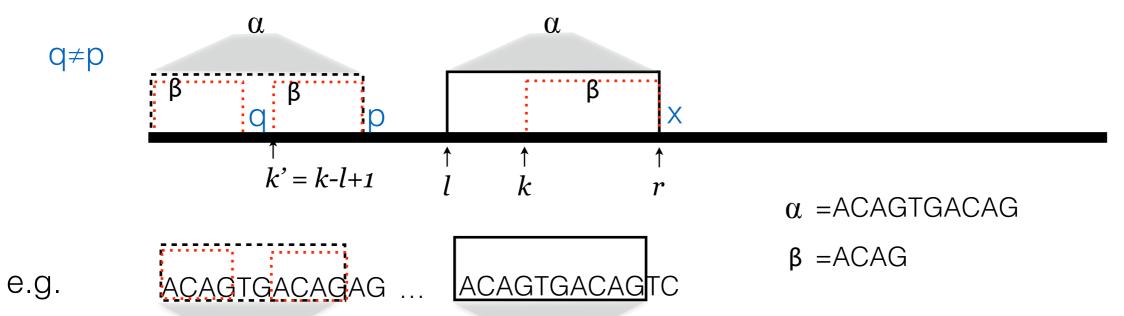
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If q = p, then  $Z_{k'}$  would have length  $> |\beta|$ 

What do we know about  $x \dots x \neq p$ . Is x = q?



#### Z Algorithm

- Input:  $Z_2...Z_{k-1}$ , and the boundaries I, r of the rightmost Z-box found starting someplace in 2...k-1.
- Output:  $Z_k$ , and updated I, r

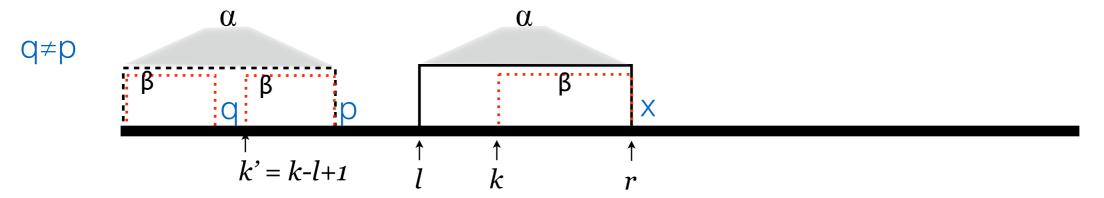
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If q = p, then  $Z_{k'}$  would have length  $> |\beta|$ 

What do we know about  $x \dots x \neq p$ . Is x = q? We don't know! Must check.



Explicitly compare after r to set  $Z_k$ . l = k, r = point where comparison failed

#### Analysis

- Correctness follows by induction and the arguments we made in the description of the algorithm.
  - If you follow all of the sub-cases, the correctness of z-alg is implied
- Runs in O(|P|+|T|) time:
  - only match characters covered by a Z-box once, so there are O(|P|+|T|) matches.
  - every iteration contains at most one mismatch, so there are O(|P|+|T|) mismatches.
- Immediately gives an O(|P| + |T|)-time algorithm for string matching as described a few slides ago.
  - O(|P| + |T|) is the best possible worst-case running time, since you might have to look at the whole input.
  - But better algorithms exist in practice that, for real instances, have expected sublinear runtime.

#### Another algorithm

The key idea here will be exploiting redundancies (i.e. self-similarities) in the pattern **P**.

Say, we have:

T = CGAGACGAGAACGAGACGAGATCCCTCTAA

P = CGAGACGAGAT

CGAGACGAGACCGAGACCGAGATCCCTCTAA IIIIIIIIIX CGAGACGAGAT

rather than shift **P** by 1 position, we can *skip* by a larger amount:

#### CGAGACGAGACCGAGATCCCTCTAA

Next possible But

occ. could stárt

here

But we know that occ. would match up until here

**Knuth**, Donald E., James H. **Morris**, Jr, and Vaughan R. **Pratt**. "Fast pattern matching in strings." SIAM journal on computing 6.2 (1977): 323-350.

The Knuth-Morris-Pratt (KMP) algorithm provides an elegant approach to exploiting this intuition, allowing us to determine the optimal "skips"

Recall the following definitions:

```
String \mathbf{s} is a prefix of \mathbf{t} if \mathbf{t} = \mathbf{s}\mathbf{u} and a suffix of \mathbf{t} if \mathbf{t} = \mathbf{u}\mathbf{s} if neither \mathbf{s} nor \mathbf{u} are \boldsymbol{\epsilon}, then \mathbf{s} is a proper prefix/suffix of \mathbf{t}
```

Main idea: Build a *partial match* table, **pm**, that tells us, for each proper **suffix** of **P[0:q]**, the length of the longest match between this **suffix** and a proper **prefix** of **P[0:q]**.

In words, pm[q] is the number for which P[0:pm[q]] is the longest proper prefix of P that is also a proper suffix of P[0:q]

Р	С	G	A	G	A	С	G	A	G	A	Т
q	0	1	2	3	4	5	6	7	8	9	10
pm[q]	0	0	0	0	0	1	2	3	4	5	0

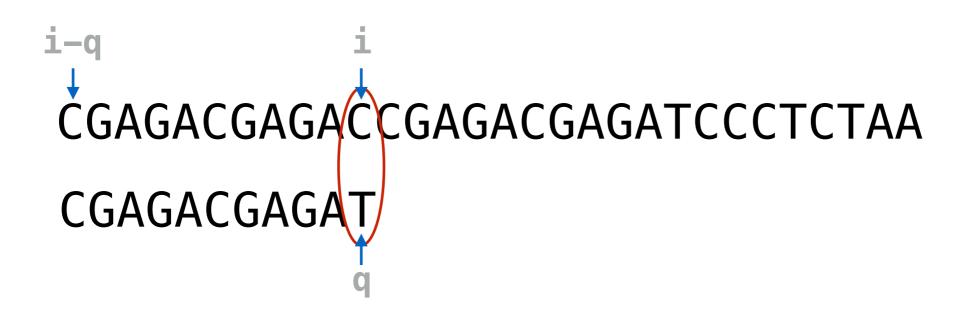
CGAGACGAGAT 00000123450

The algorithm progresses as follows, assuming that P[0:q-1] matches T[i-q-1: i-1]:

If P[q] = T[i], then if q < m we extend the length of the match, otherwise we've found a match and set q = pm[q-1]

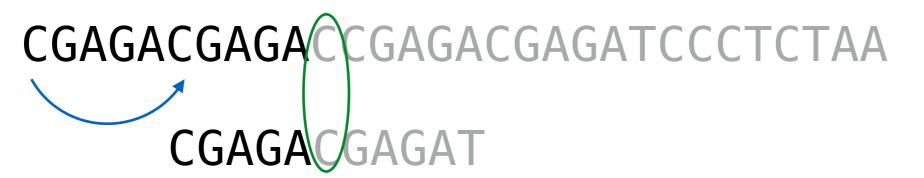
Else P[q]  $\neq$ T[i], then if q = 0 we increment i, otherwise we *shift* the pattern so by pm[q-1], and set q = pm[q-1]

CGAGACGAGAT 00000123450



 $T[i=10] \neq P[q=10]$ , so we shift the pattern to the right by pm[9] = 5 and set q = pm[q-1]

 $T[i=10] \neq P[q=10]$ , so we shift the pattern to the right setting q = pm[q-1] = 5



Not only are we shifting the pattern right here, we actually skip even more character comparisons because we *begin* comparing the shifted pattern at position q = 5

CGAGACGAGAT 00000123450 i-q i 5- m

CGAGACGAGAT

C = C, so shift q and i

i-q i CGAGACGAGACCGAGACCCTCTAA

CGAGACGAGAT

 $T[i=11] \neq P[q=6]$ , so we shift the pattern so that we next compare T[i] with P at q = pm[q-1] = 1

CGAGACGAGAT 00000123450

i-q i CGAGACGAGACCGAGACCCTCTAA

CGAGACGAGAT

 $T[i=11] \neq P[q=6]$ , so we shift the pattern so that we next compare T[i] with P at q = pm[q-1] = 1

i-q i
CGAGACGAGACCGAGACCCTCTAA

CGAGACGAGAT

 $T[i=11] \neq P[q=1]$ , so we shift the pattern so that we next compare T[i] with P at q = pm[q-1] = 0

CGAGACGAGAT 00000123450

i-q i
CGAGACGAGACCGAGACCCTCTAA

CGAGACGAGAT

 $T[i=11] \neq P[q=1]$ , so we shift the pattern so that we next compare T[i] with P at q = pm[q-1] = 0

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT 00000123450

Now we continue advancing by 1 ... for a while

CGAGACGAGAT CCCTCTAA

CGAGACGAGAT

CGAGACGAGAT 00000123450

CGAGACGAGAC CGAGACGAGAT CCCTCTAA

Found a match; set q = pm[q-1] = pm[9] = 5

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT

 $T[i=21] \neq P[q=5]$ , so we shift the pattern so that we next compare T[i] with P at q = pm[q-1] = 0

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT

CGAGACGAGACCGAGACGAGATCCCTCTAA

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT

CGAGACGAGACCGAGATCCCTCTAA

**CGAGACGAGAT** 

q

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGACCAGATCCCTCTAA

CGAGACGAGAT

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGACCAGATCCCTCTAA

**CGAGACGAGAT** 

q

i

CGAGACGAGACCGAGACCCTCTAA

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT

q

CGAGACGAGACCGAGATCCCTCTAA



CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT

CGAGACGAGACCGAGATCCCTCTAA

**CGAGACGAGAT** 

q

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

**CGAGACGAGAT** 

q

CGAGACGAGACCGAGATCCCTCTAA

**CGAGACGAGAT** 

q

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

**CGAGACGAGAT** 

q



CGAGACGAGACCGAGACCCTCTAA



CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

**CGAGACGAGAT** 

q

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT 00000123450

CGAGACGAGACCGAGATCCCTCTAA

CGAGACGAGAT

CGAGACGAGACCGAGATCCCTCTAA

#### KMP code

```
def kmp(P,T):
    n = len(T)
    m = len(P)
    matches = []
    pi = partialMatchTable(P)
    q = 0
    i = 0
    while i < n:</pre>
        if P[q] == T[i]:
            q += 1
            i += 1
             if q == m:
                 matches.append(i-q)
                 q = pi[q-1]
        else:
             if q == 0:
               i += 1
             else:
                 q = pi[q-1]
    return matches
```

#### Running Time

Each pass through the outer loop either increments i or shifts the pattern to the right.

Both of these events can occur at most n times, and so, the loop, in total, can execute at most 2n = O(n) times.

Assuming **pm** is precomputed, each event takes O(1) time.

Computing pm takes O(m) time — we'll see that next

KMP runs in O(n+m) time

#### Computing the Partial Match Table

The key to the linearity of partialMatchTable() is that we always use pm[0:i] to compute pm[i+1]

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 0

q = 1

Р	С	G	A	G	A	С	G	A	G	A	т
q	0	1									
pm[q]	0	0									

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 0

q = 2q = 2

P	С	G	A	G	A	С	G	A	G	A	т
q	0	1	2								
pm[q]	0	0	0								

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 0

q = 3 q = 3

Р	С	G	A	G	A	С	G	A	G	A	Т
q	0	1	2	3							
pm[q]	0	0	0	0							

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 0

P	С	G	A	G	A	С	G	A	G	A	т
q	0	1	2	3	4						
pm[q]	0	0	0	0	0						

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 0

loop end: m = 11 k = 1

q = 5q = 5

P	С	G	A	G	A	С	G	A	G	A	Т
q	0	1	2	3	4	5					
pm[q]	0	0	0	0	0	1					

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 1

q = 6 q = 6

P	С	G	A	G	A	С	G	A	G	A	т
q	0	1	2	3	4	5	6				
pm[q]	0	0	0	0	0	1	2				

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 2

loop end: m = 11 k = 3

q = 7 q = **7** 

Р	C	G	A	G	A	С	G	A	G	A	Т
q	0	1	2	3	4	5	6	7			
pm[q]	0	0	0	0	0	1	2	3			

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 3

q = 8

loop end: m = 11 k = 4

q = 8

Р	C	G	A	G	A	С	G	A	G	A	Т
q	0	1	2	3	4	5	6	7	8		
pm[q]	0	0	0	0	0	1	2	3	4		

```
def partialMatchTable(p):
   m = len(p)
    pm = [0] * m
    k = 0
    for q in range(1, m):
        while k > 0 and p[k] != p[q]:
            k = pm[k - 1]
        if p[k] == p[q]:
           k = k + 1
        pm[q] = k
    return pm
```

k = 4

loop end: m = 11 k = 5

q = 9q = 9

Р	C	G	A	G	A	С	G	A	G	A	Т
q	0	1	2	3	4	5	6	7	8	9	
pm[q]	0	0	0	0	0	1	2	3	4	5	

k = 5

q = 10

loop end: m = 11

k = 0

q = 10

Р	С	G	A	G	A	С	G	A	G	A	т
q	0	1	2	3	4	5	6	7	8	9	10
pm[q]	0	0	0	0	0	1	2	3	4	5	0

#### Summary

Despite our ability to solve general pairwise alignment, exact matching is still important

The naive algorithm for the problem takes O(MN) time

By exploiting structure in the *pattern*, we reduce the worst case runtime to O(M+N)

Dan Gusfield is awesome!

Knuth, Morris & Pratt are awesome!

Next time, we'll see how to do even better by preprocessing the *text*.