EMS-GT2: An Improved Exact Solution for the (l, d)-Planted Motif Problem

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1. Context of the Study
2. Definition of Terms
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Context of the Study

Context

Motif Finding

Given a set of DNA sequences, find common substrings in each sequence considering a number of allowed mutations

Context

(l, d)-planted motif search problem

*Given a set of **n** sequences with length of **m** each, find the planted motif of length **l** considering up to **d** mutations:*

(l, d)-planted motif problem:

Ex: ***n = 4 m = 30 l = 5 d = 2***

S1 taagctgctattctacggatagatactaca

S2 acacttgactatatataggatctaggatacat

S3 actagatatacctataggcacattgctgga

S4 tagagcacatagacctgacacatagtactt

Find the planted motif M: ***?***

(l, d)-planted motif problem:

Ex: ***n = 4   m = 30   l = 5   d = 2***

S1 taagctgcta**ttcta**cggatagatactaca

S2 a**cactt**gactatataggatctaggatacat

S3 actagatatacctataggcacat**tgctg**ga

S4 tagagcacatag**acctg**acacatagtactt

Find the planted motif M: ***tactg***

Definition of terms

Definition of Terms

***l*-mer:**

- a string of length l in the alphabet Σ

in this context we use Σ = {a, c, g, t}

Definition of Terms

motif:

- *l*-mer that occurs across different sequences (but with subject to mutations)

Definition of Terms

dH(x,y)**: hamming distance**

- the number of mismatch positions between two l-mers.

ex: dH(actg, gcta) = 2

Definition of Terms

d-neighbor of an l-mer x:

- is another *l*-mer ***y*** whose hamming distance with ***x*** is at most **d**.

Definition of Terms

N(x, d): ***d-neighborhood of an l-mer x:***

- is the set of all *l*-mers with at most *d* hamming distance value from *x*.

Definition of Terms

N(x, d): ***d-neighborhood of an l-mer x:***

Example: l = 4, d = 2

gatc

{

**a**a**a**c, **a**a**c**c, **a**a**g**c, **a**at**a**, **a**atc, **a**at**g**, **a**at**t**, **ac**tc, **ag**tc, **at**tc,

**c**a**a**c, **c**a**c**c, **c**a**g**c, **c**at**a**, **c**atc, **c**at**g**, **c**at**t**, **cc**tc, **cg**tc, **ct**tc,

_ga**aa**, ga**a**c, ga**ag**, ga**at**, ga**ca**, ga**c**c, ga**cg**, ga**ct**, ga**ga**,_

ga**g**c, ga**gg**, ga**gt**, ga**ta**, gatc, gat**g**, gat**t**, g**ca**c, g**cc**c,

_g**cg**c, g**c**t**a**, g**c**tc, g**c**t**g**, g**c**t**t**, g**ga**c, g**gc**c, g**gg**c, g**g**t**a**,_

_g**g**tc, g**g**t**g**, g**g**t**t**, g**ta**c, g**tc**c, g**tg**c, g**t**t**a**, g**t**tc, g**t**t**g**, g**t**t**t**,_

**t**a**a**c, **t**a**c**c, **t**a**g**c, **t**at**a**, **t**atc, **t**at**g**, **t**at**t**, **tc**tc, **tg**tc, **tt**tc

}

Definition of Terms

N(*S, d*)***: d-neighborhood of a sequence S***

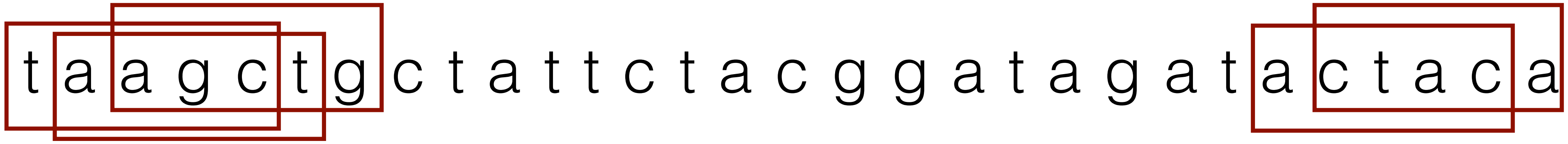
- is the set of all d-neighbors of all l-mers in sequence S.

- there are exactly *(m - l +1) l*-mers in sequence S of length m.

Definition of Terms

N*(S, d)****: d-neighborhood of a sequence S***

l = 5

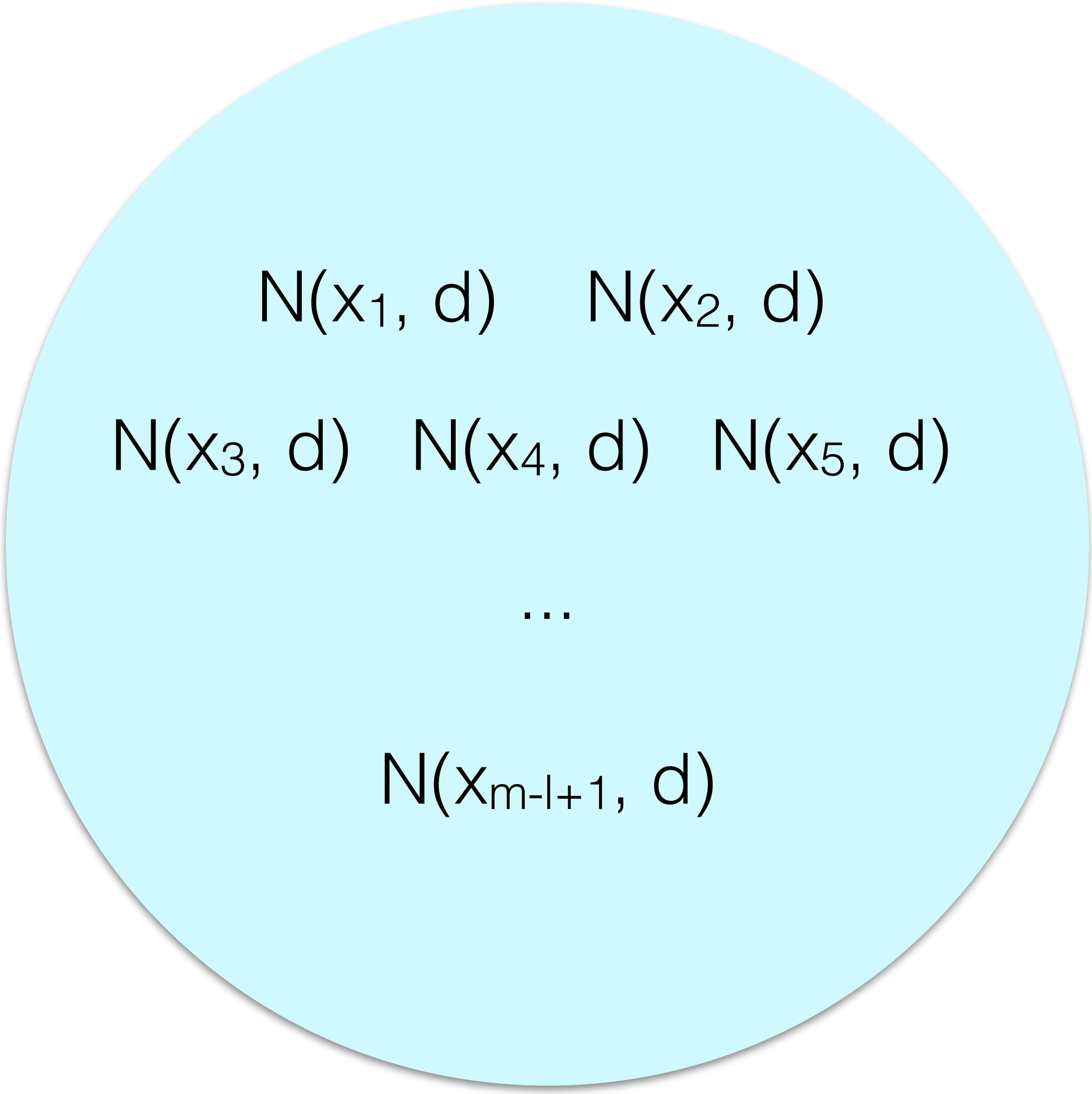


S1 taagctgctattctacggatagatactaca

Definition of Terms

N**(S, d)*: ***d*-neighborhood of a sequence *S

***N**(S, d)* =



$N(x_1, d)$ $N(x_2, d)$

$N(x_3, d)$ $N(x_4, d)$ $N(x_5, d)$

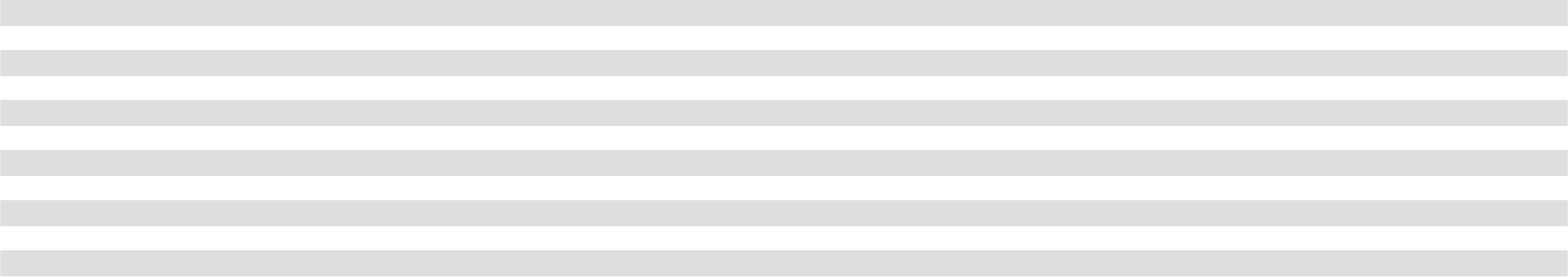
...

$N(x_{m-l+1}, d)$

EMS-GT Algorithm

First Approach:

It checks every possible combination of positions in different sequences and tests if it is the correct position where the motif is planted.



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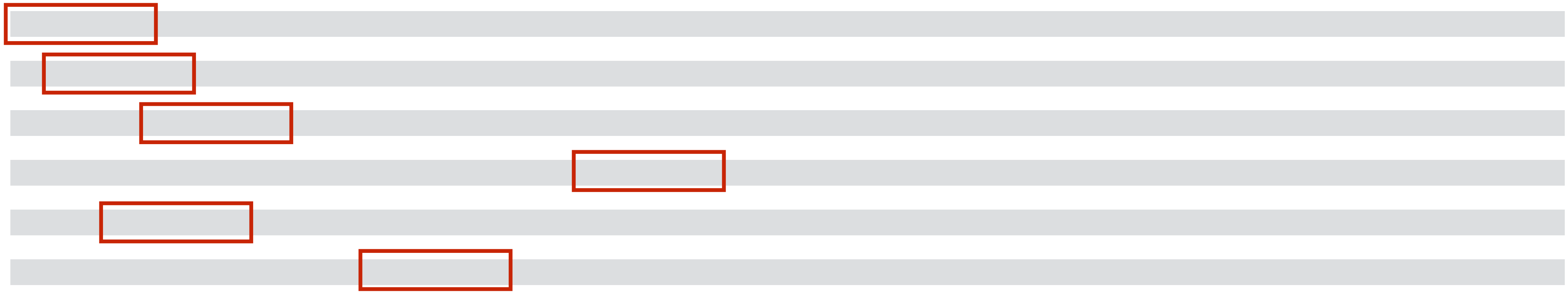

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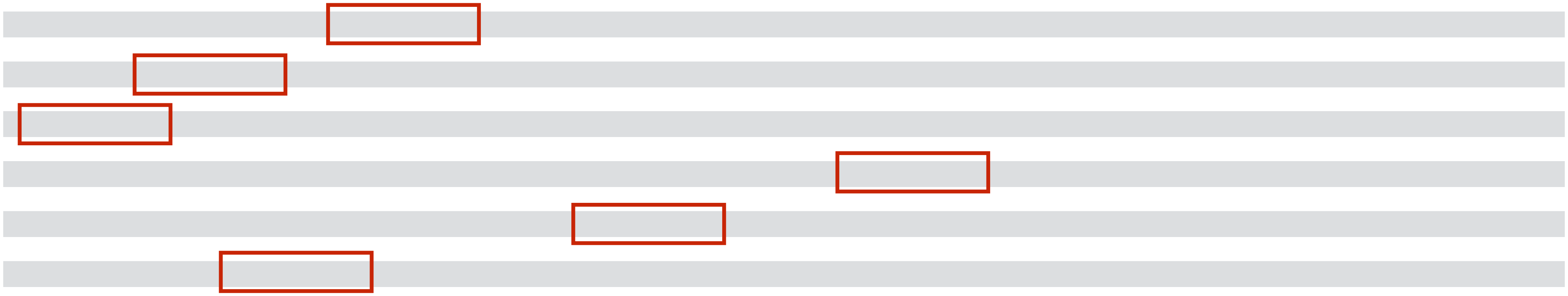


Second Approach:

Exhaustively searches all possible 4^l l-mers if it a motif.

4^l possible l-mers

Exact Motif Search - Generate and Test (EMS-GT)

EMS-GT is composed of 2 phases.

Generate Phase: quickly filters the search space by doing a set intersection between the d-neighborhood of the first n' sequences. Resulting set is the candidate motif set.

Test Phase: evaluates each candidate motif if it has at least one d-neighbor in the remaining (n - n') sequences.

EMS-GT: Demonstration:

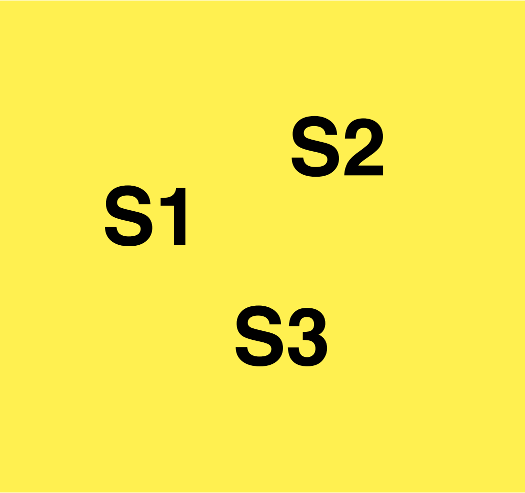
Parameters	$n = 5$	$m = 30$	$l = 5$	$d = 2$	$n' = 3$
Dataset	**S1**	**S2**	**S3**	**S4**	**S5**

EMS-GT: Demonstration:

Parameters $n = 5$ $m = 30$ $l = 5$ $d = 2$ $n' = 3$

Dataset **S1** **S2** **S3** **S4** **S5**

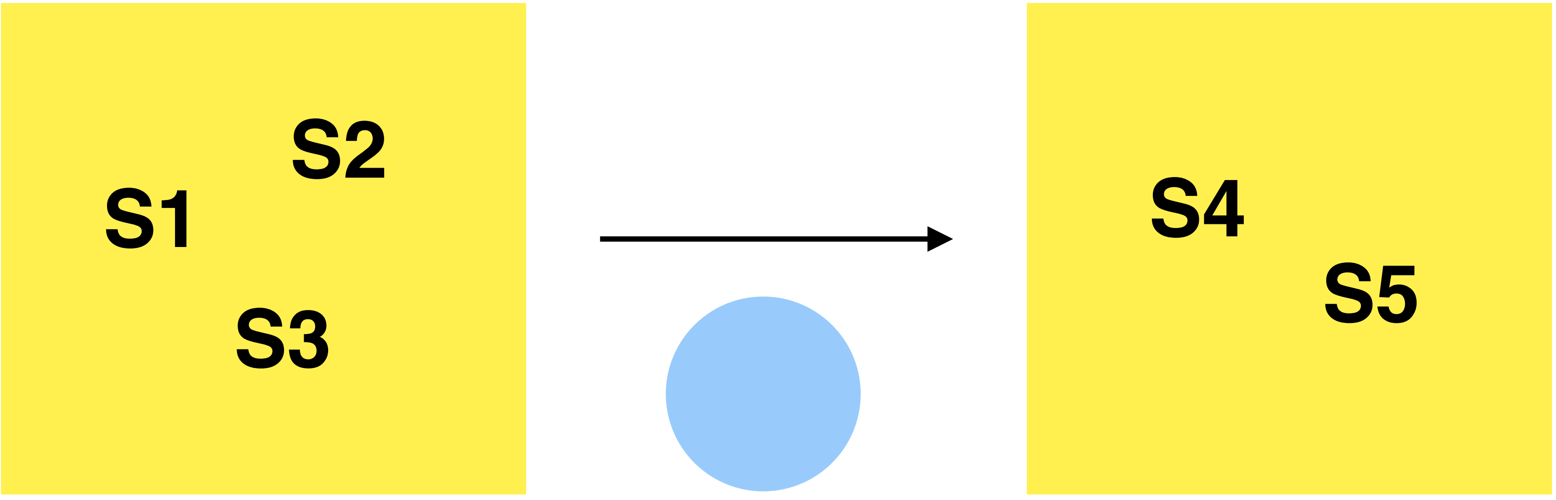
Generate



EMS-GT: Demonstration:

Parameters $n = 5$ $m = 30$ $l = 5$ $d = 2$ $n' = 3$

Dataset **S1 S2 S3 S4 S5**



Generate

S1 S2 S3

Test

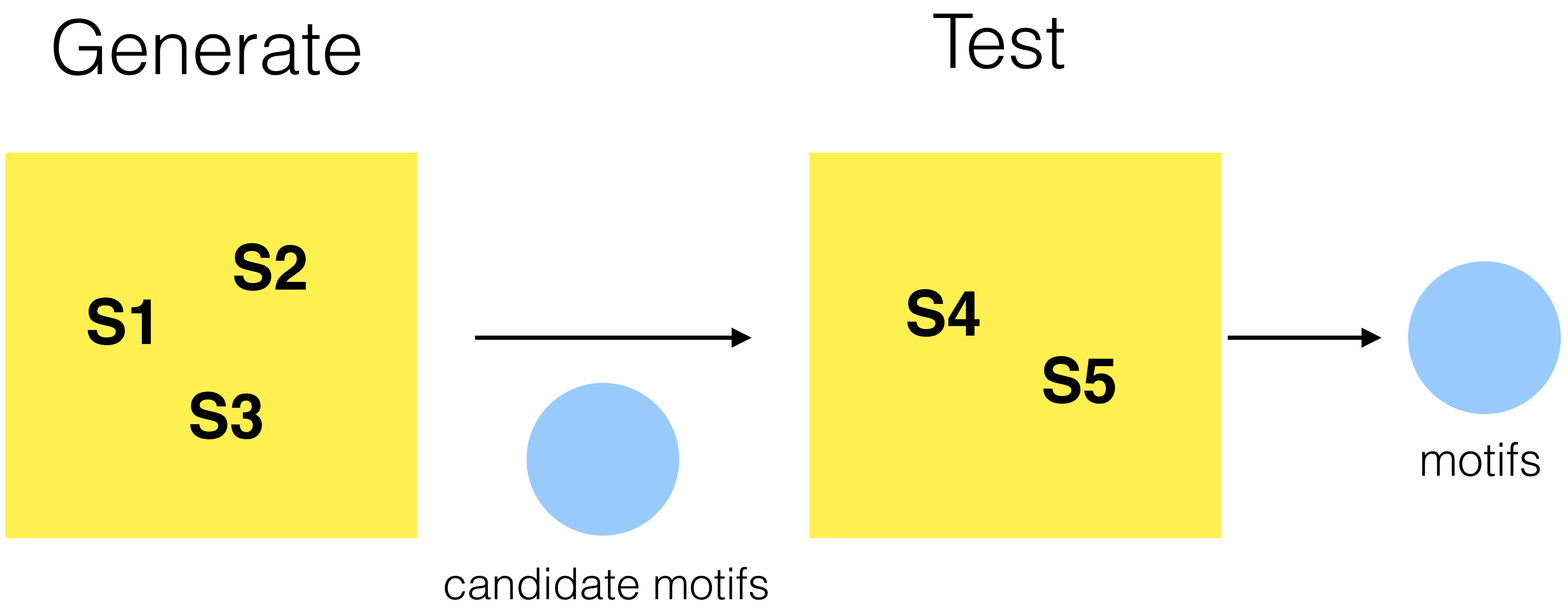
S4 S5

candidate motifs

EMS-GT: Demonstration:

Parameters $n = 5$ $m = 30$ $l = 5$ $d = 2$ $n' = 3$

Dataset **S1 S2 S3 S4 S5**



Generate

Test

S1 **S2** **S3**

candidate motifs

S4 **S5**

motifs

Generate Phase

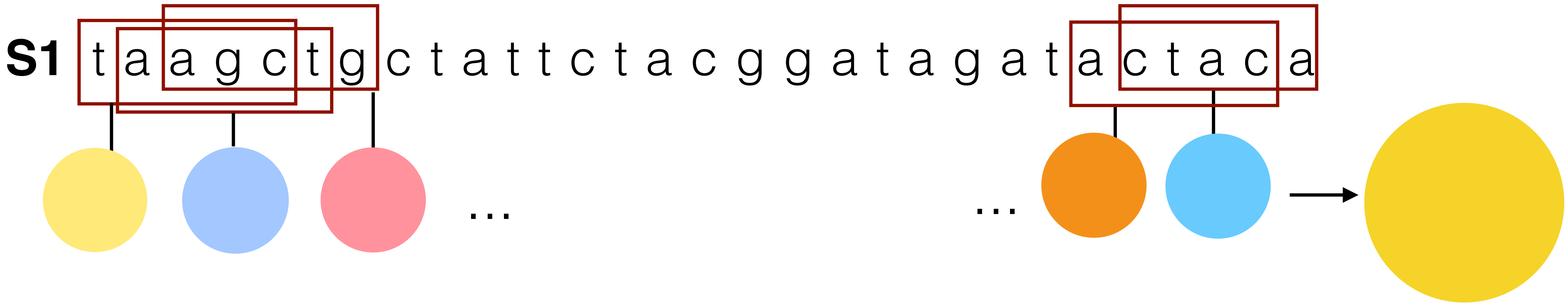
$n = 5$ $m = 30$ $l = 5$ $d = 2$ $n' = 3$

S1 t a a g c t g c t a t t c t a c g g a t a g a t a c t a c a

S2 a c a c t t g a c t a t a t a g g a t c t a g g a t a c a t

Generate Phase

***n* = 5 *m* = 30 *l* = 5 *d* = 2 *n'* = 3**

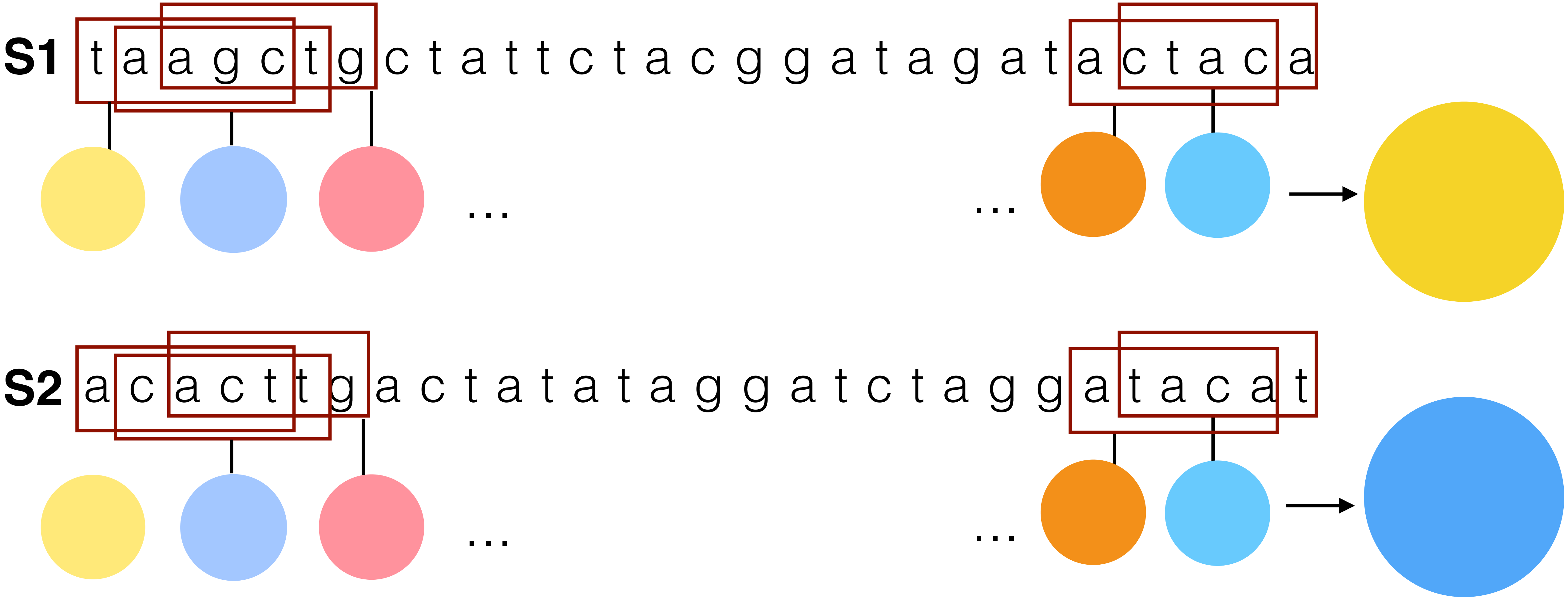


S1 t a a g c t g c t a t t c t a c g g a t a g a t a c t a c a

S2 a c a c t t g a c t a t a t a g g a t c t a g g a t a c a t

Generate Phase

***n* = 5 *m* = 30 *l* = 5 *d* = 2 *n'* = 3**

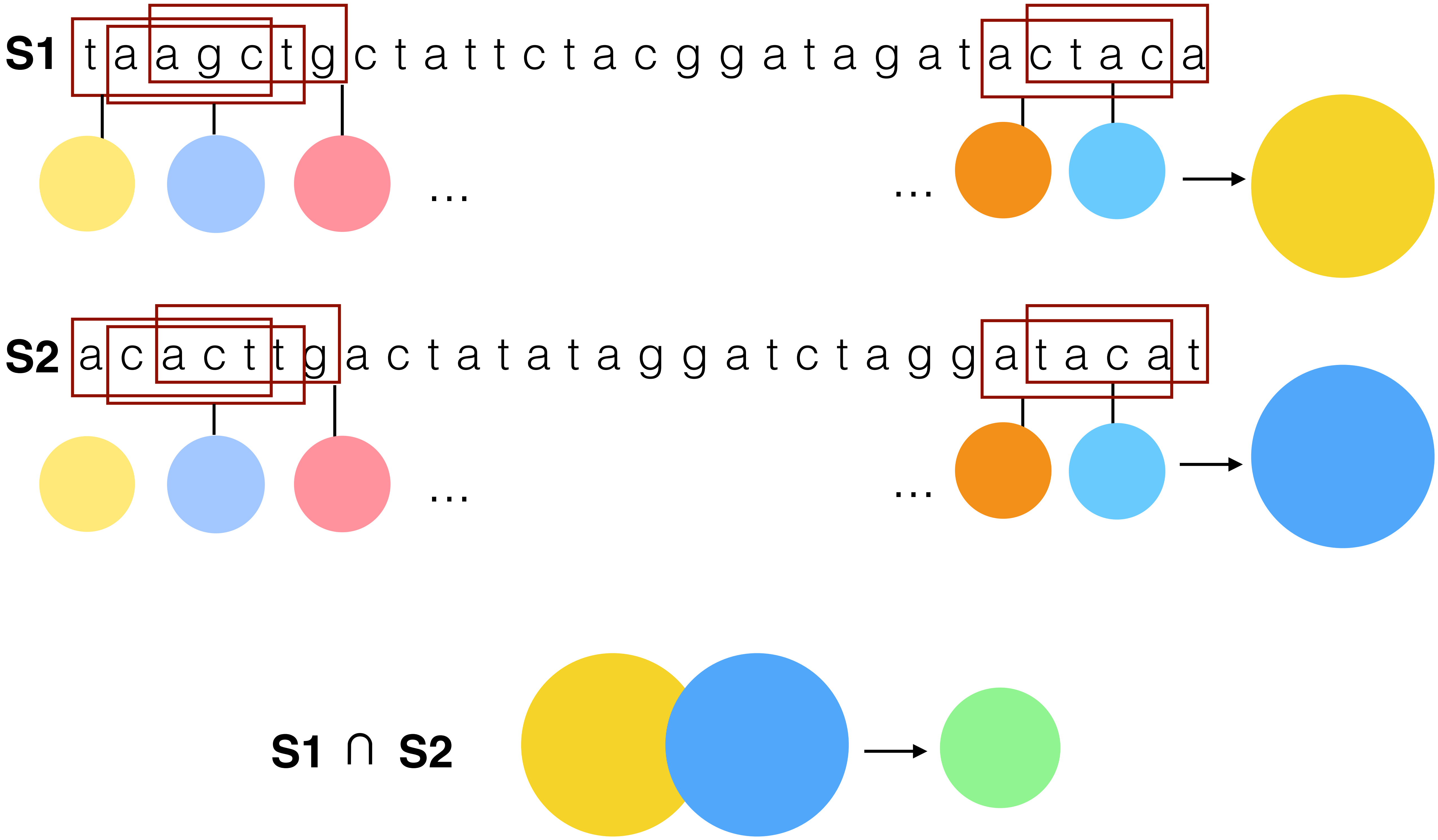


S1 taagctgctattctacggatagatactaca … …

S2 acacttgactatataggatctaggatacat … …

Generate Phase

***n* = 5 *m* = 30 *l* = 5 *d* = 2 *n'* = 3**



S1 taagctgctattctacggatagatactaca

…

…

S2 acacttgactatataggatctaggatacat

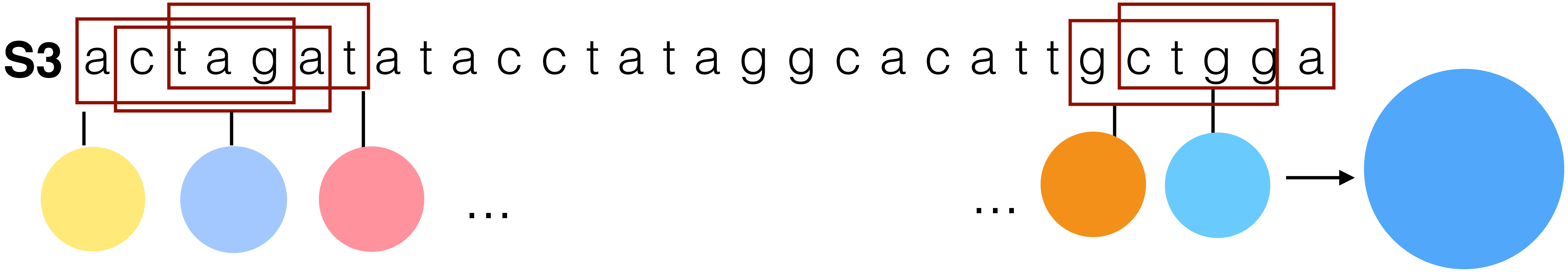
…

…

S1 ∩ S2

Generate Phase

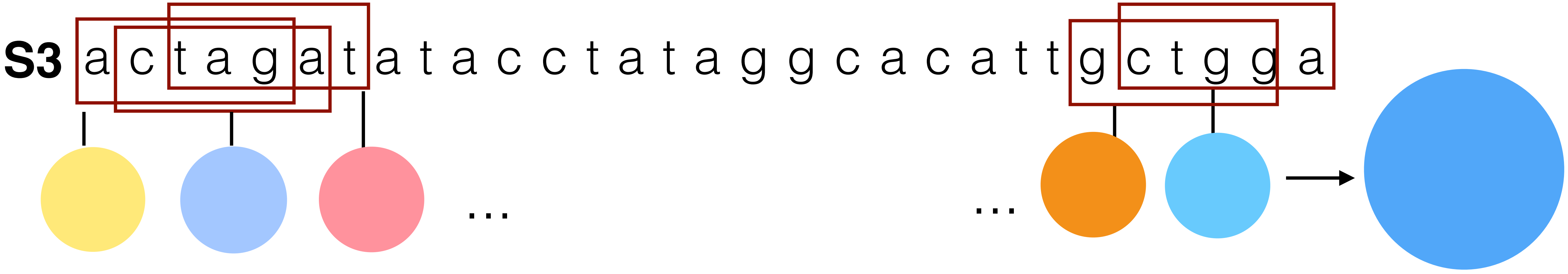
n = 5   m = 30   l = 5   d = 2   n' = 3



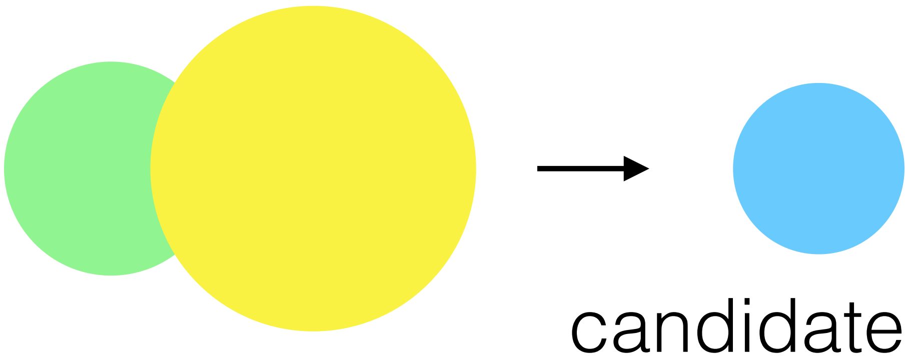
S3 a c t a g a t a t a c c t a t a g g c a c a t t g c t g g a

Generate Phase

***n* = 5 *m* = 30 *l* = 5 *d* = 2 *n'* = 3**



S1 ∩ S2 ∩ S3

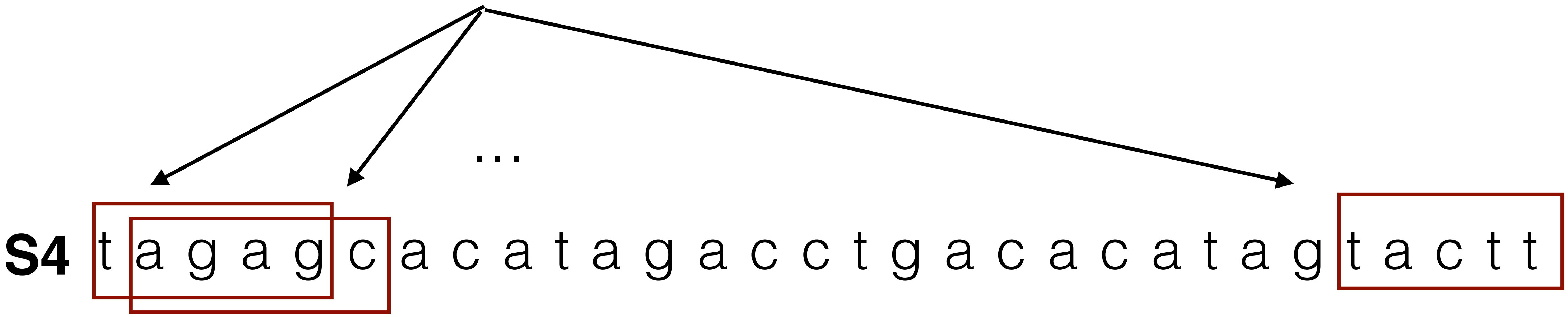


candidate motifs

EMS-GT: Demonstration: ***n = 5 m = 30 l = 5 d = 2 n' = 2***

Test Phase:

candidate motifs = {tagac, ccatg, tagtt}



S4 t a g a g c a c a t a g a c c t g a c a c a t a g t a c t t

S5 c a g a t a g a c t a t a g g c c a t a t a c c g t a g a a

EMS-GT: Demonstration: ***n* = 5 *m* = 30 *l* = 5 *d* = 2 *n'* = 2**

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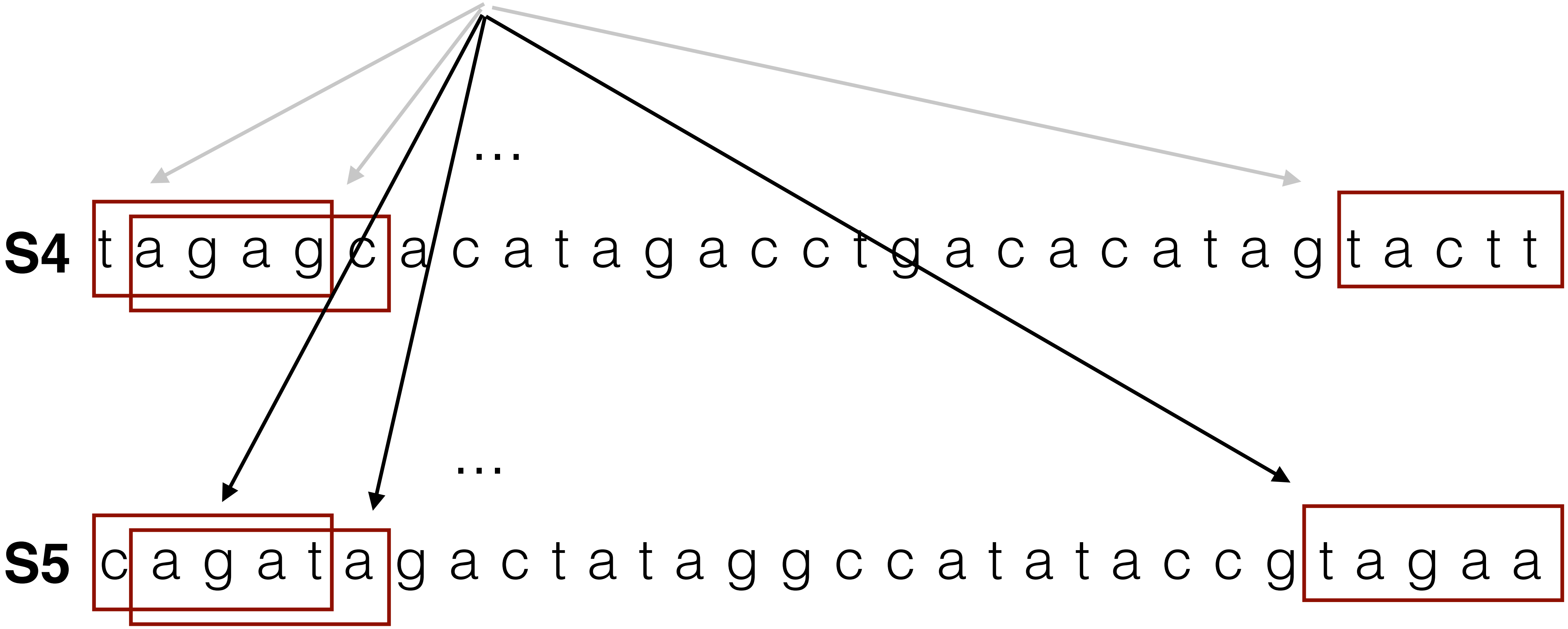


...

S4 t a g a g c a c a t a g a c c t g a c a c a t a g t a c t t

...

S5 c a g a t a g a c t a t a g g c c a t a t a c c g t a g a a

Implementation

Implementation: Speedup Techniques

1. Integer Mapping of an *l*-mer

a = 00 | c = 01 | g = 10 | t =11

example:

tacgt is mapped to 1100011011

integer value = 795

Implementation: Speedup Techniques

2. Bit-based set representation and l-mer enumeration

Set Representation

0	0
1	1
2	1
3	0
⋮	
4^l	0

We know that there are ***4^l*** *number of possible l-mers given the DNA bases.*

A value of ***1*** *means it is in the set while* ***0*** *means otherwise*

Implementation: Speedup Techniques

2. Bit-based set representation and l-mer enumeration

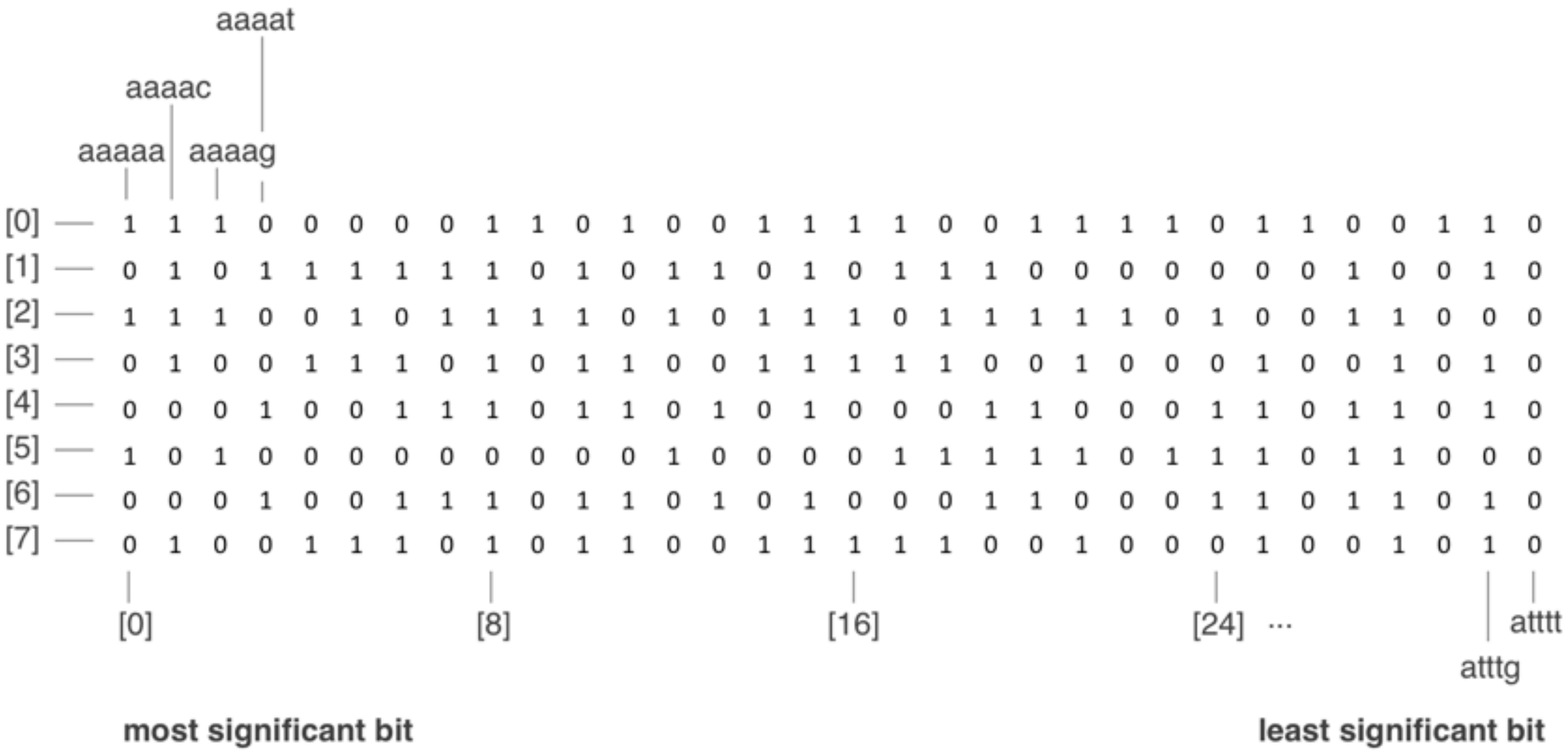
Set Representation

0	0
1	1
2	1
3	0
⋮	
4^l	0

*In this example we know that l-mers with value of **1** and **2** belong to the set.*

1 = AAAAC and 2 = AAAAG, if l = 5

3. Bit-array compression



	aaaaa	aaaac	aaaag	aaaat																												
[0]	1	1	1	0	0	0	0	0	1	1	0	1	0	0	1	1	1	1	0	0	1	1	1	1	0	1	1	0	0	1	1	0
[1]	0	1	0	1	1	1	1	1	1	0	1	0	1	1	0	1	0	1	1	1	0	0	0	0	0	0	0	1	0	0	1	0
[2]	1	1	1	0	0	1	0	1	1	1	1	0	1	0	1	1	1	0	1	1	1	1	1	0	1	0	0	1	1	0	0	0
[3]	0	1	0	0	1	1	1	0	1	0	1	1	0	0	1	1	1	1	1	0	0	1	0	0	0	1	0	0	1	0	1	0
[4]	0	0	0	1	0	0	1	1	1	0	1	1	0	1	0	1	0	0	0	1	1	0	0	0	1	1	0	1	1	0	1	0
[5]	1	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1	1	1	1	1	0	1	1	1	0	1	1	0	0	0
[6]	0	0	0	1	0	0	1	1	1	0	1	1	0	1	0	1	0	0	0	1	1	0	0	0	1	1	0	1	1	0	1	0
[7]	0	1	0	0	1	1	1	0	1	0	1	1	0	0	1	1	1	1	1	0	0	1	0	0	0	1	0	0	1	0	1	0
	[0]								[8]								[16]								[24]	···					atttg	atttt

most significant bit

least significant bit

Implementation: Speedup Techniques

3. Bit-array compression

** each element contains a 32-bit integer for bit flags instead of one.*

Implementation: Speedup Techniques

3. Bit-array compression

** the process of setting and checking the value:*

gacgt = 1000011011 = **539** in decimal

bit position = 539 mod 32 = 27;

array index = 539 / 32 = 16;

*The bit flag for **gacgt** is in the 27th least significant bit of the integer at array index 16.*

Implementation: Speedup Techniques

4. XOR-based Hamming distance computation

Example:

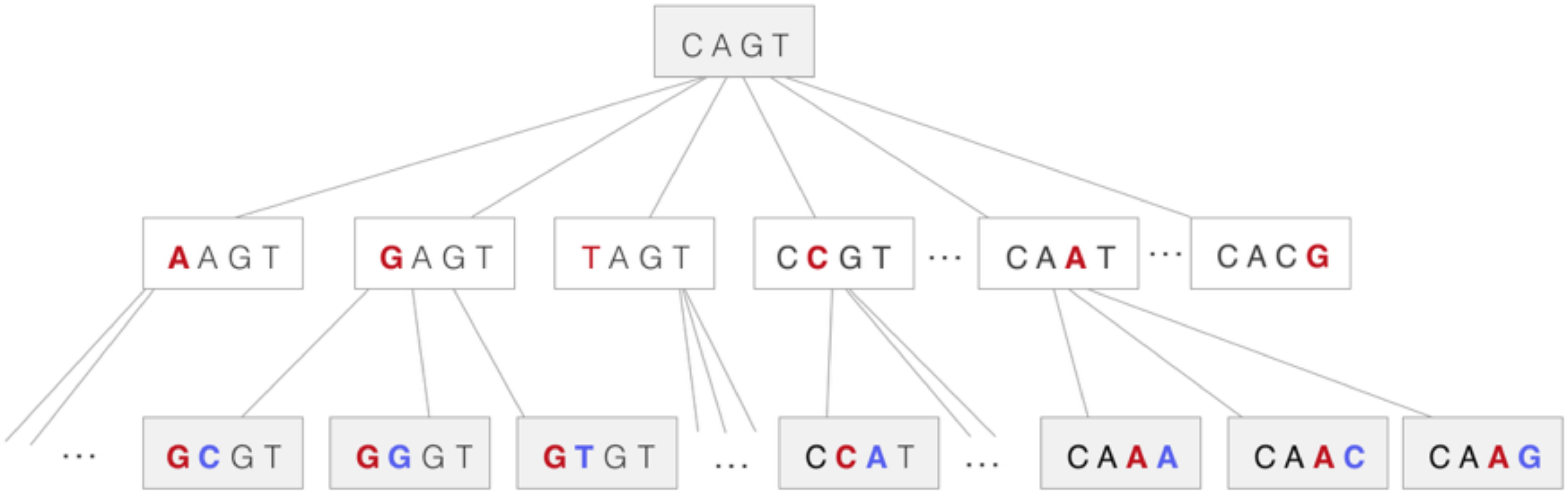
aacgt maps to 0000011011

tacgc maps to 1100011001

XOR produces 1100000010 *= 2 mismatches*

Implementation: Speedup Techniques

5. Recursive neighborhood generation



Implementation: Speedup Techniques

6. Block-based optimization for neighborhood generation

- *instead of setting one bit at a time in the neighborhood generation, we generate the neighborhood by blocks*

Implementation: Speedup Techniques

6. Block-based optimization for neighborhood generation

- *instead of setting one bit at a time in the neighborhood generation, we generate the neighborhood by blocks*

- *if we partition the bit-array N into* ***4^k*** *of bits, where $k < l$, each block will conform to one of* ***(k + 2) patterns.***

Implementation: Speedup Techniques

6. Block-based optimization for neighborhood generation

- instead of setting one bit at a time in the neighborhood generation, we generate the neighborhood by blocks

- if we partition the bit-array N into ***4^k*** *of bits, where k < l, each block will conform to one of* ***(k + 2) patterns.***

- we pre-computed these ***block patterns*** *and use it to set the bits in the bit-array by blocks.*

Implementation: Speedup Techniques

6. Block-based optimization for neighborhood generation

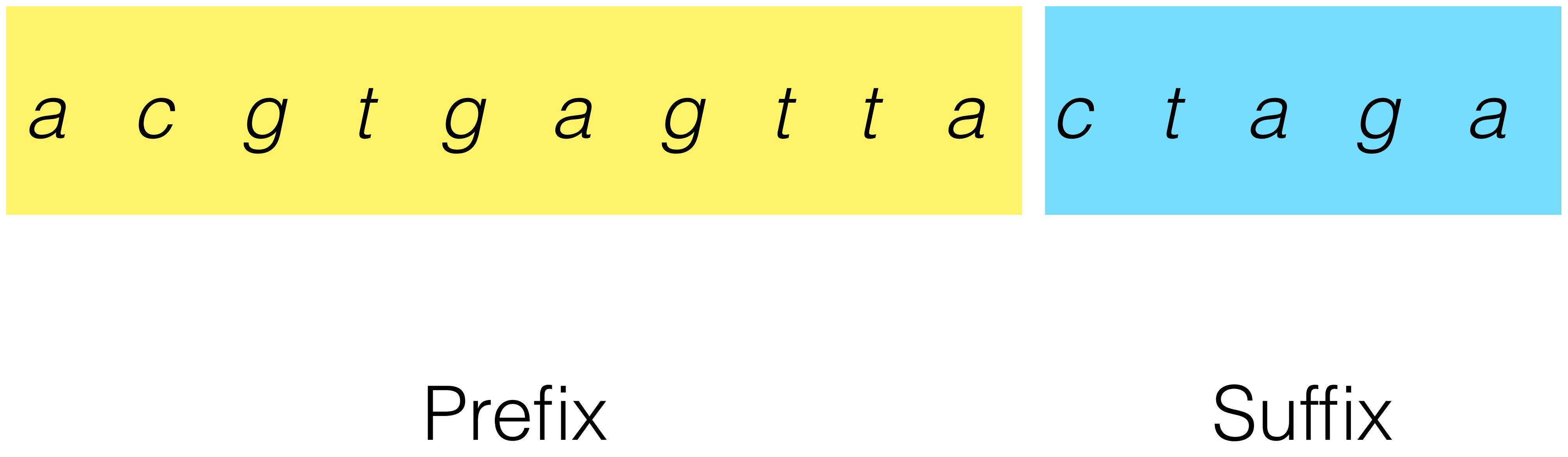
Lets say we want to generate the d-neighborhood of 15-mer

a c g t g a g t t a c t a g a

Implementation: Speedup Techniques

6. Block-based optimization for neighborhood generation

Lets say we want to generate the d-neighborhood of 15-mer



a c g t g a g t t a *c t a g a*

Prefix Suffix

Implementation: Speedup Techniques

6. Block-based optimization for neighborhood generation

Now instead of recursively generating all d-neighbor of length ***l****, we only consider up to (l-k) prefix of l. For each prefix, we apply the corresponding block pattern based on the remaining allowed mutations.*

Additional Speedup Techniques

1. Faster Candidate Motif Elimination through Block Processing.

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Observations:

- The bit array that stores the candidate motifs is enumerated alphabetically.

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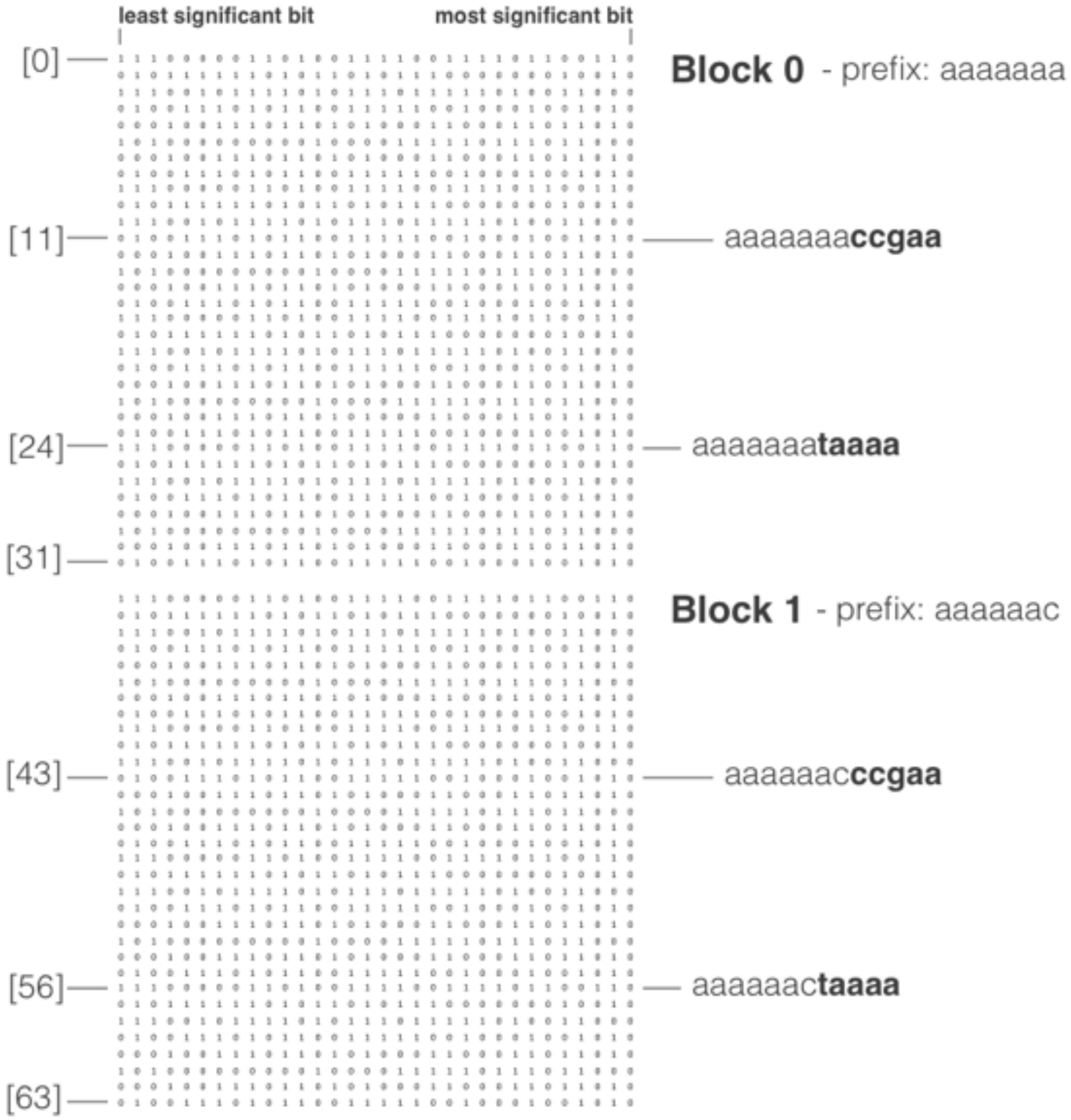
- The bit array that stores the candidate motifs is enumerated alphabetically.

- Given the alphabetical enumeration, *l*-mers near other do not differ that much.

- In EMS-GT, each candidate motif testing is independent of other.

Faster Candidate Motif Elimination through Block Processing.



least significant bit

most significant bit

[0] — **Block 0** - prefix: aaaaaaa

[11] — aaaaaaa**ccgaa**

[24] — aaaaaaa**taaaa**

[31]

Block 1 - prefix: aaaaaac

[43] — aaaaaac**ccgaa**

[56] — aaaaaac**taaaa**

[63]

By grouping every 4^k bits into blocks, we can exploit some of the blocks' properties.

Faster Candidate Motif Elimination through Block Processing.

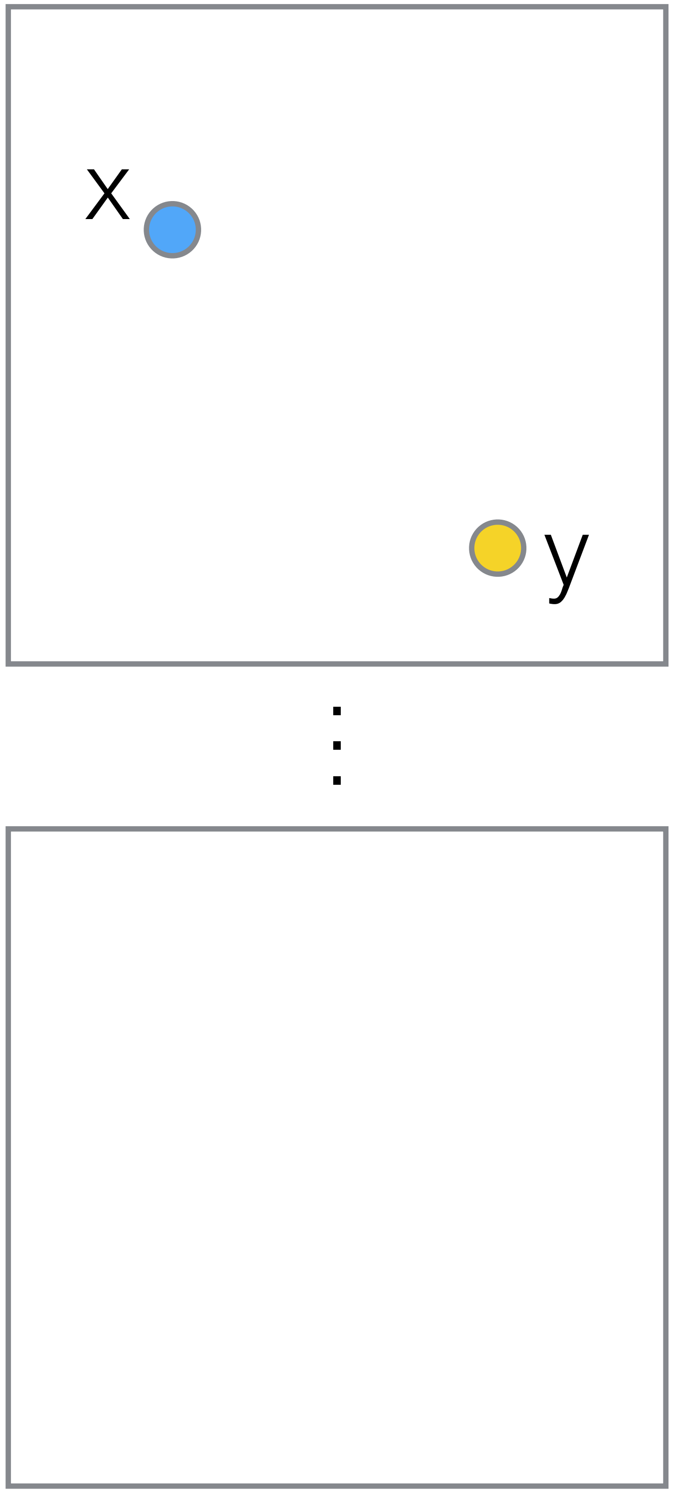
By grouping every 4^k bits into blocks, we can derive these properties:

- *Each l-mer in a block shares the same prefix string.*
- *For every block, the hamming distance of any two l-mers is at most k.*

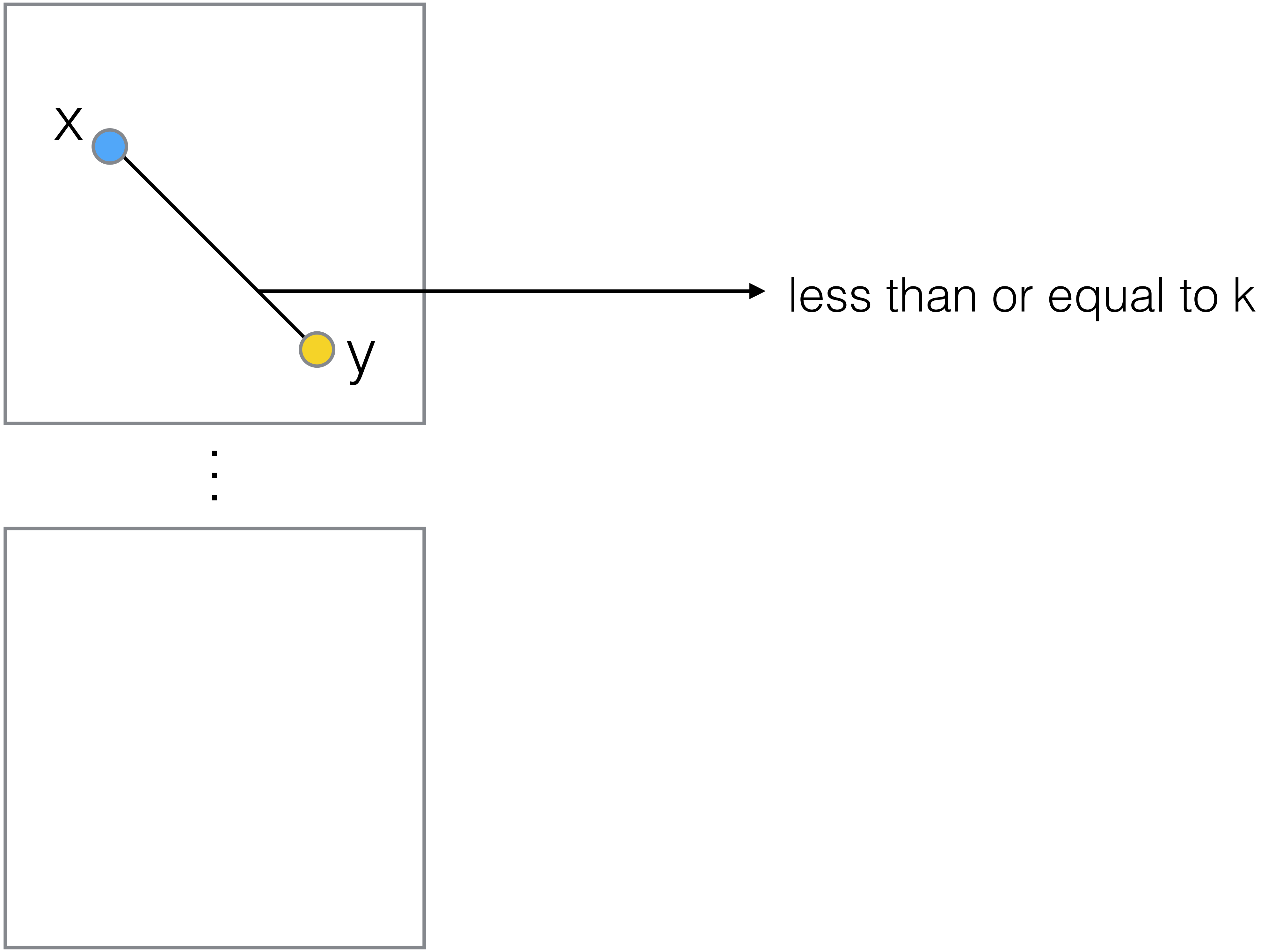
Faster Candidate Motif Elimination through Block Processing.

Theorem. *Let x and y be l-mers in a block in the search space containing 4^k l-mers. Let d be the number of allowed mutations in the problem instance. Let z be another l-mer. If $dH(x, z) > (k + d)$ then $dH(y, z) > d$, and therefore z is not in $N(y, d)$*

Faster Candidate Motif Elimination through Block Processing.



Faster Candidate Motif Elimination through Block Processing.



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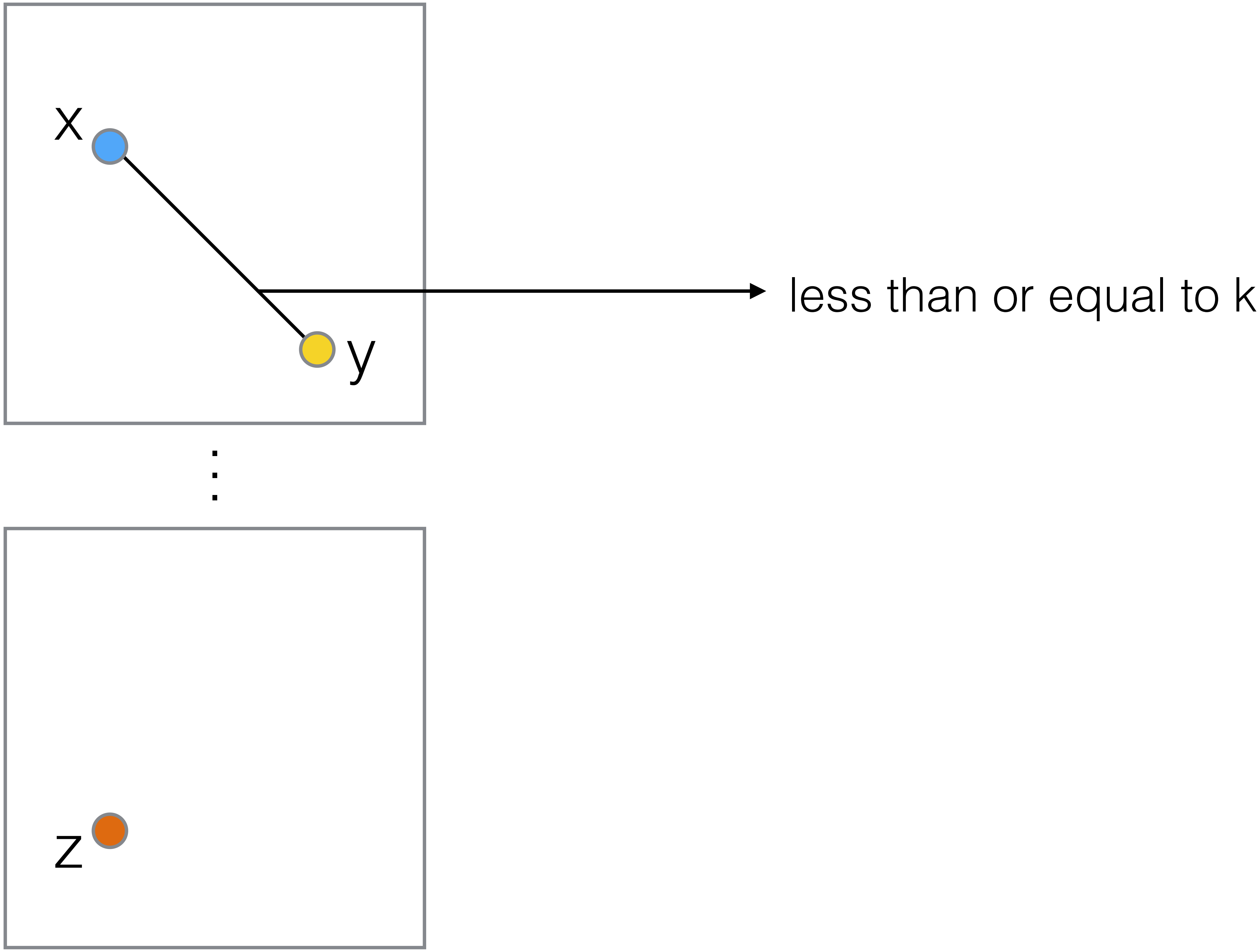

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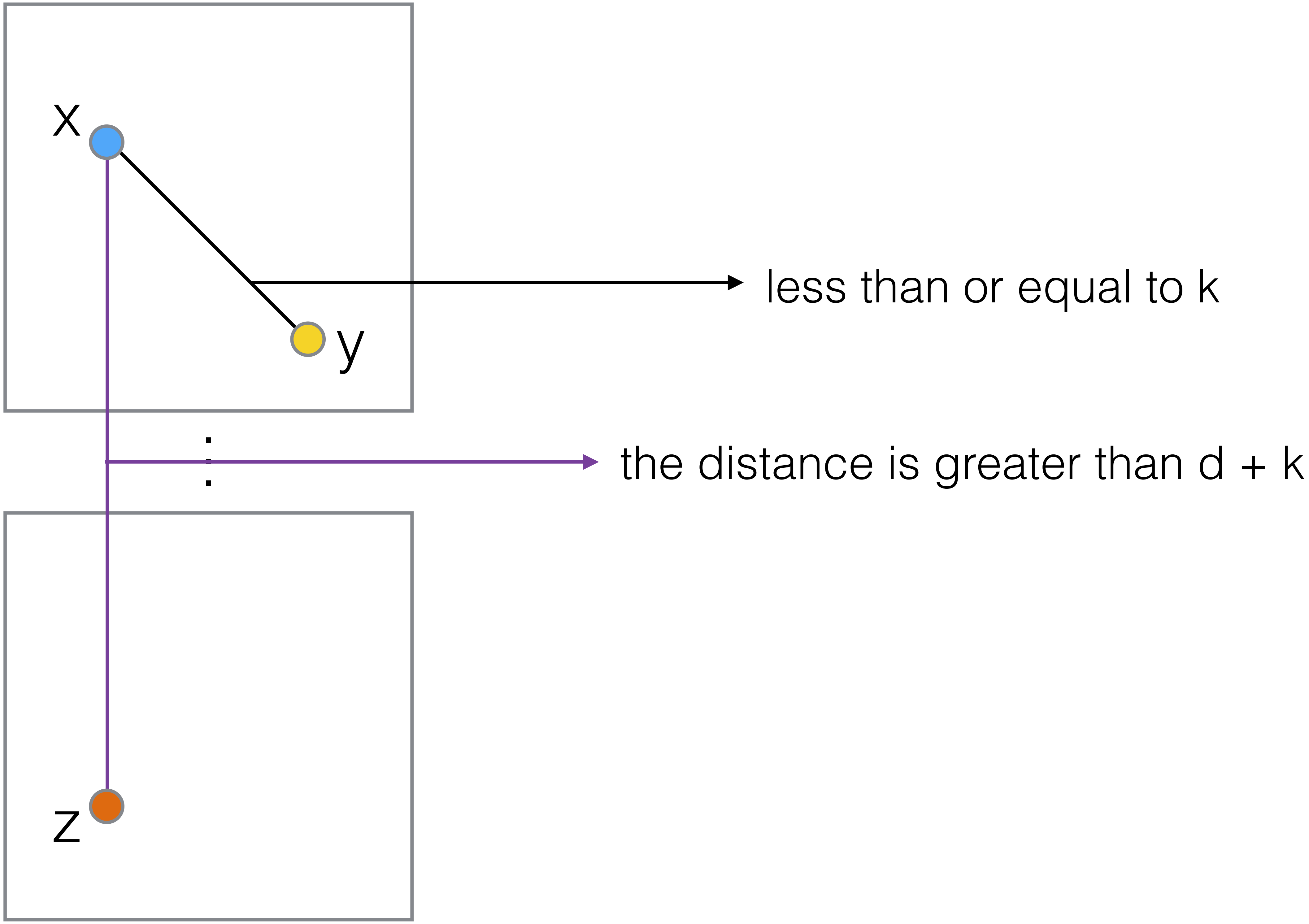
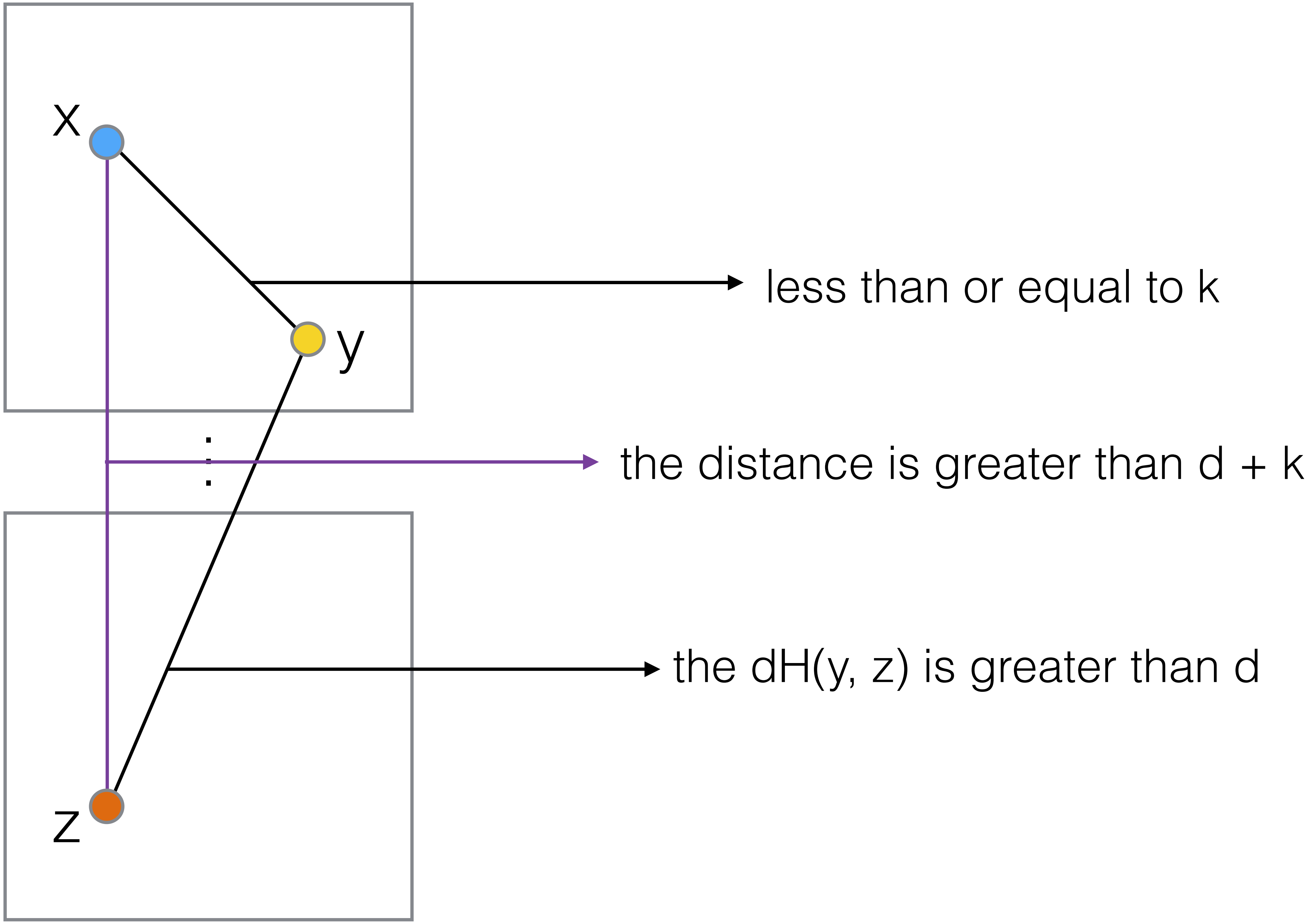


less than or equal to k

the distance is greater than d + k

Faster Candidate Motif Elimination through Block Processing.



less than or equal to k

the distance is greater than d + k

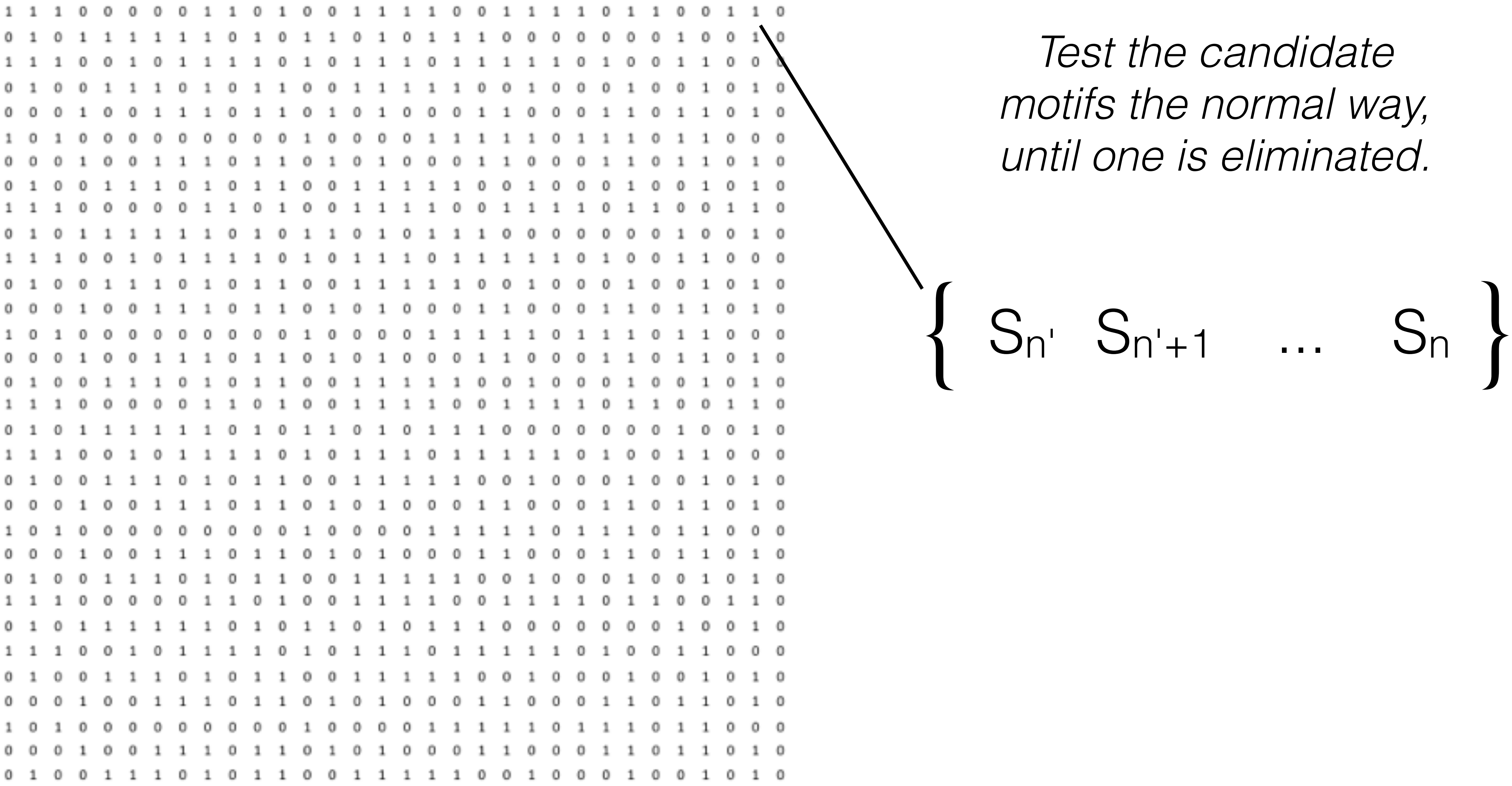
the dH(y, z) is greater than d

Faster Candidate Motif Elimination through Block Processing.

We used this theorem in the Test Phase by filtering some of the l-mers in a sequence S.

Faster Candidate Motif Elimination through Block Processing.

Improved Test Phase:



```
1 1 1 0 0 0 0 0 1 1 0 1 0 0 1 1 1 1 0 0 1 1 1 1 0 1 1 0 0 1 1 0
0 1 0 1 1 1 1 1 1 0 1 0 1 1 0 1 0 1 1 1 0 0 0 0 0 0 0 1 0 0 1 0
1 1 1 0 0 1 0 1 1 1 1 0 1 0 1 1 1 0 1 1 1 1 1 0 1 0 0 1 1 0 0 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
1 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 1 1 1 1 0 1 1 1 0 1 1 0 0 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
1 1 1 0 0 0 0 0 1 1 0 1 0 0 1 1 1 1 0 0 1 1 1 1 0 1 1 0 0 1 1 0
0 1 0 1 1 1 1 1 1 0 1 0 1 1 0 1 0 1 1 1 0 0 0 0 0 0 0 1 0 0 1 0
1 1 1 0 0 1 0 1 1 1 1 0 1 0 1 1 1 0 1 1 1 1 1 0 1 0 0 1 1 0 0 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
1 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 1 1 1 1 0 1 1 1 0 1 1 0 0 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
1 1 1 0 0 0 0 0 1 1 0 1 0 0 1 1 1 1 0 0 1 1 1 1 0 1 1 0 0 1 1 0
0 1 0 1 1 1 1 1 1 0 1 0 1 1 0 1 0 1 1 1 0 0 0 0 0 0 0 1 0 0 1 0
1 1 1 0 0 1 0 1 1 1 1 0 1 0 1 1 1 0 1 1 1 1 1 0 1 0 0 1 1 0 0 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
1 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 1 1 1 1 0 1 1 1 0 1 1 0 0 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
1 1 1 0 0 0 0 0 1 1 0 1 0 0 1 1 1 1 0 0 1 1 1 1 0 1 1 0 0 1 1 0
0 1 0 1 1 1 1 1 1 0 1 0 1 1 0 1 0 1 1 1 0 0 0 0 0 0 0 1 0 0 1 0
1 1 1 0 0 1 0 1 1 1 1 0 1 0 1 1 1 0 1 1 1 1 1 0 1 0 0 1 1 0 0 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
1 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 1 1 1 1 0 1 1 1 0 1 1 0 0 0
0 0 0 1 0 0 1 1 1 0 1 1 0 1 0 1 0 0 0 1 1 0 0 0 1 1 0 1 1 0 1 0
0 1 0 0 1 1 1 0 1 0 1 1 0 0 1 1 1 1 1 0 0 1 0 0 0 1 0 0 1 0 1 0
```

Test the candidate motifs the normal way, until one is eliminated.

$$\left\{ S_{n'} \quad S_{n'+1} \quad \dots \quad S_{n} \right\}$$

Faster Candidate Motif Elimination through Block Processing.

Improved Test Phase:

gagct

$\mathbf{S_{n''}}$ t a g a g c a c a t a g a c c t g a c a c a t a g t a c t t

↓ l-mers in sequence Sn''

{ tagag, agagc, gagca, agcac ... tactt }

Faster Candidate Motif Elimination through Block Processing.

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$S_{n''}$ t a g a g c a c a t a g a c c t g a c a c a t a g t a c t t

↓ l-mers in sequence Sn''

{ tagag, ~~agagc,~~ gagca, ~~agcac~~ ... tactt }

we can filter some l-mers in the set of (m-l+1) l-mers of Sn''
where the candidate motif got eliminated

Faster Candidate Motif Elimination through Block Processing.

*We now use this **filtered** set of l-mers over the original sequence for testing the remaining candidate motifs in the block.*

2. Pre-computation of Mismatch values for Hamming distance Computation

2. Pre-computation of Mismatch values for Hamming distance Computation

Example:

aacgt maps to 0000011011
tacgc maps to 1100011001

XOR produces 1100000010 *= 2 mismatches*

2. Pre-computation of Mismatch values for Hamming distance Computation

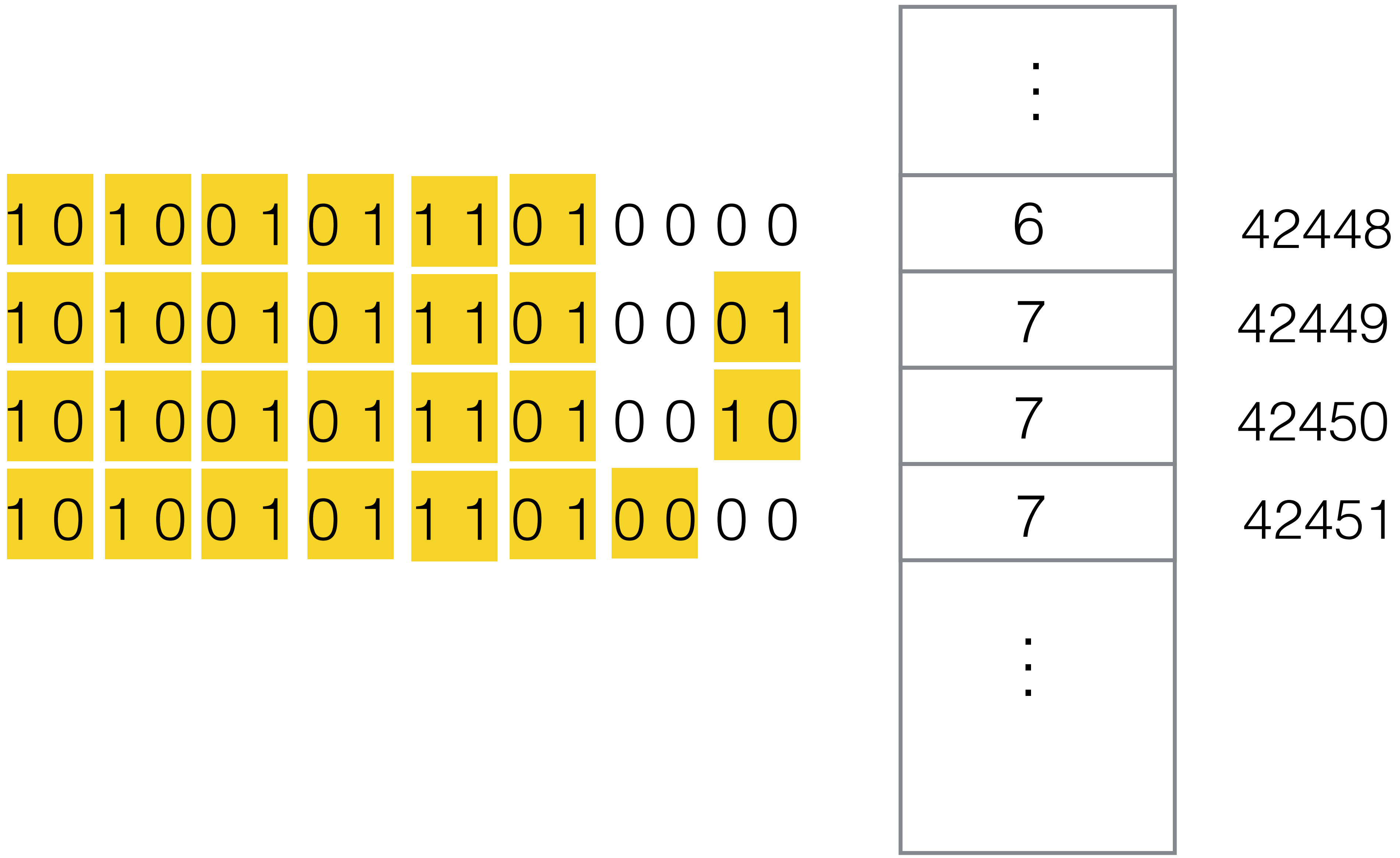
Originally, EMS-GT counts each pairs of bits in the XOR result for the Hamming distance computation.

2. Pre-computation of Mismatch values for Hamming distance Computation

We can improve this by referring to a pre-computed mismatch count values instead of counting the pair of bits every Hamming distance computation.

Pre-computation of Mismatch values

The pre-computed array of mismatch values lookup



	⋮	
1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0	6	42448
1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 1	7	42449
1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 0	7	42450
1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0	7	42451
	⋮	

Pre-computation of Mismatch values

Improved Hamming distance computation:

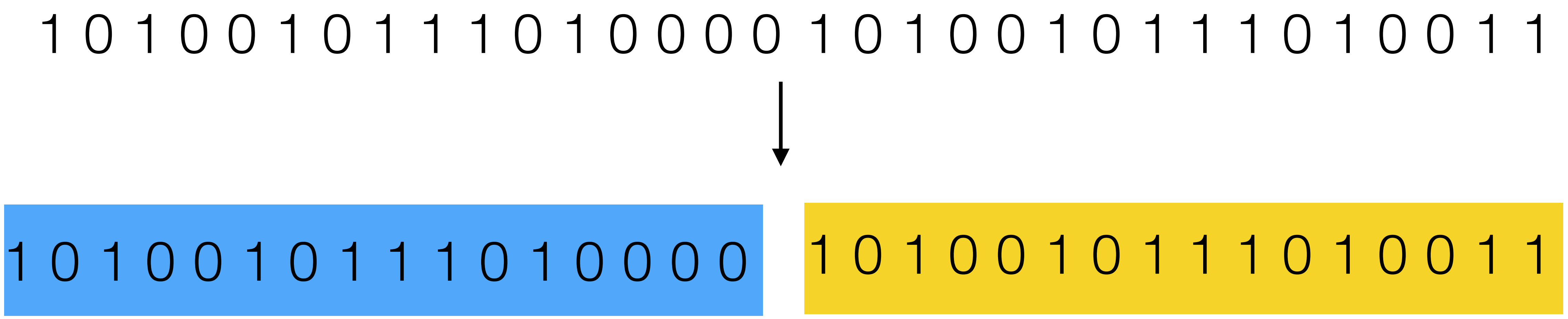
Example: Given a pre-computed values up to 16-bits and an XOR result:

1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0 1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 1

Pre-computation of Mismatch values

Improved Hamming distance computation:

Example: Given a pre-computed values up to 16-bits and an XOR result:



1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0 1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 1

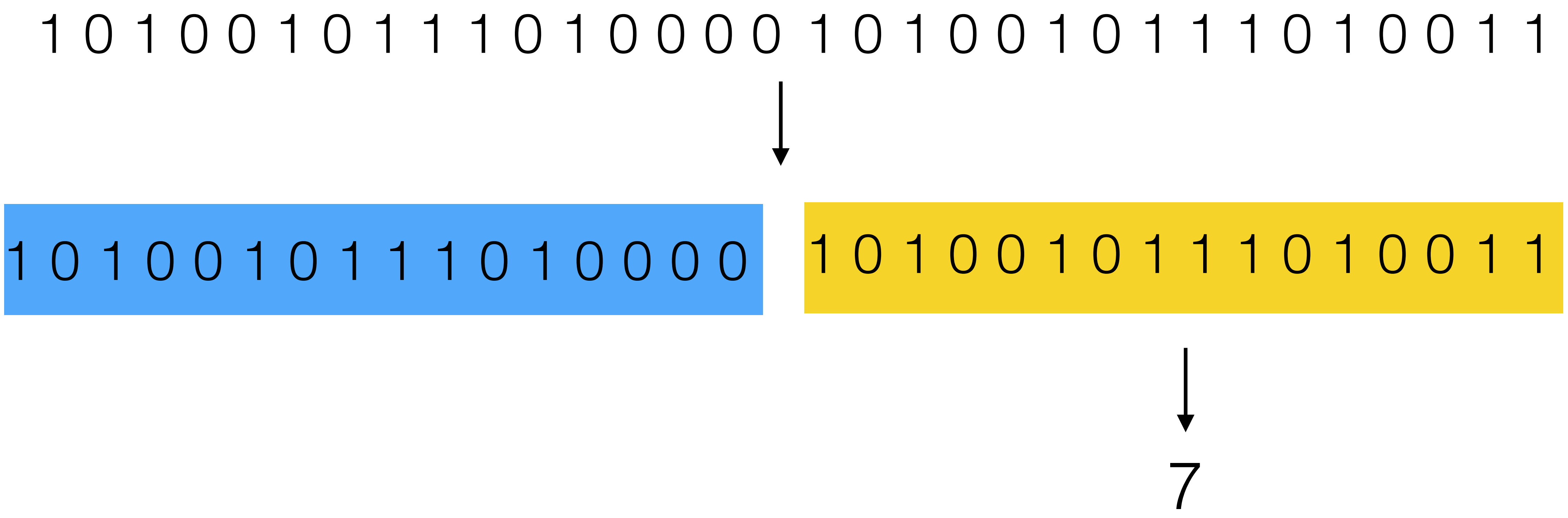
1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0

1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 1

Pre-computation of Mismatch values

Improved Hamming distance computation:

Example: Given a pre-computed values up to 16-bits and an XOR result:



1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0 1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 1

1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0

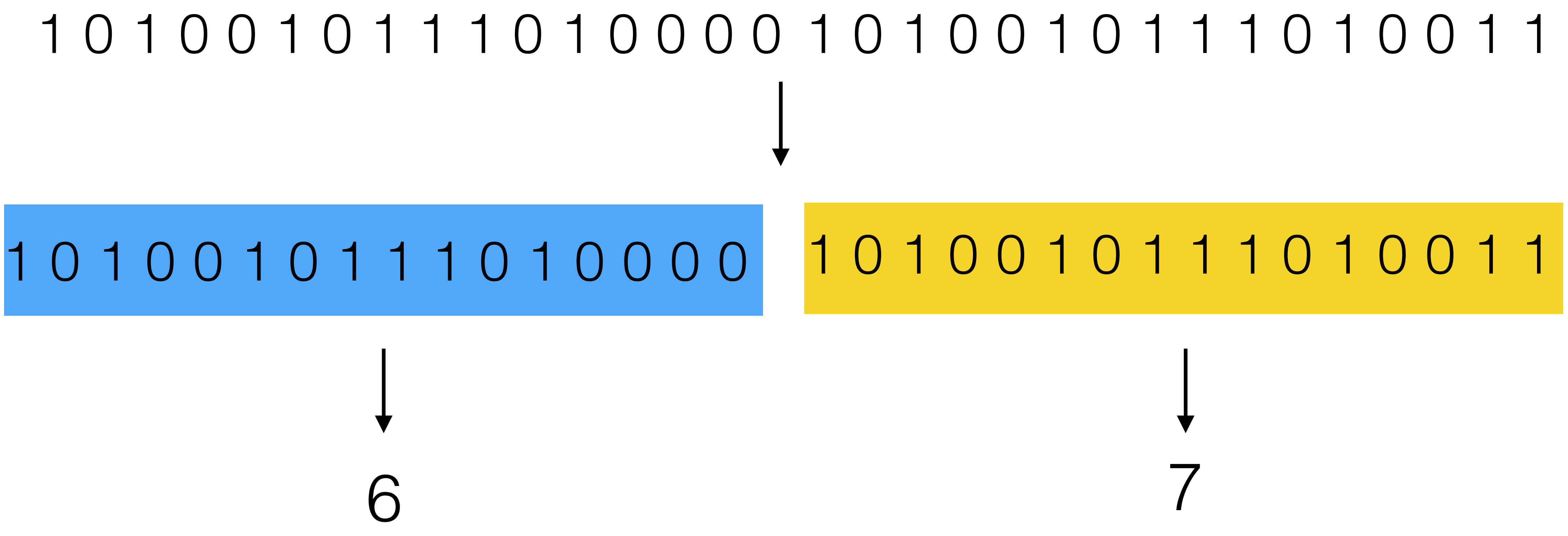
1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 1

7

Pre-computation of Mismatch values

Improved Hamming distance computation:

Example: Given a pre-computed values up to 16-bits and an XOR result:



1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0 1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 1

1 0 1 0 0 1 0 1 1 1 0 1 0 0 0 0

1 0 1 0 0 1 0 1 1 1 0 1 0 0 1 1

6

7

6 + 7 = 13 the hamming distance is **13**

Methods

Methods

Dataset

20 DNA sequences (n)

each sequence is 600 characters long (m)

used (l, d)-challenge instances, where l < 18.

Methods

Evaluation

Runtime evaluation of EMS-GT, qPMS9 and EMS-GT2 using ***(9, 2), (11, 3), (13, 4), (15, 5) and (17, 6)*** *challenge instances over 20 iterations each.*

Performance

Performance:

Experimentation Results:

	qPMS9	EMS-GT	EMS-GT2
(9, 2)	0.60 s	**0.04 s**	0.05 s
(11, 3)	1.26 s	**0.17 s**	0.26 s
(13, 4)	4.58 s	1.03 s	**0.82 s**
(15, 5)	25.73 s	12.39 s	**10.43 s**
(17, 6)	123.17 s	143.87 s	**111.22 s**

Conclusions:

EMS-GT2 is efficient in finding short motifs
where l < 18

EMS-GT2 proved its competitiveness by beating
qPMS9 in all (l, d)-challenge instances
where l < 18.

In practice, motifs are typically 10 base pairs.