

Chapter 12.6

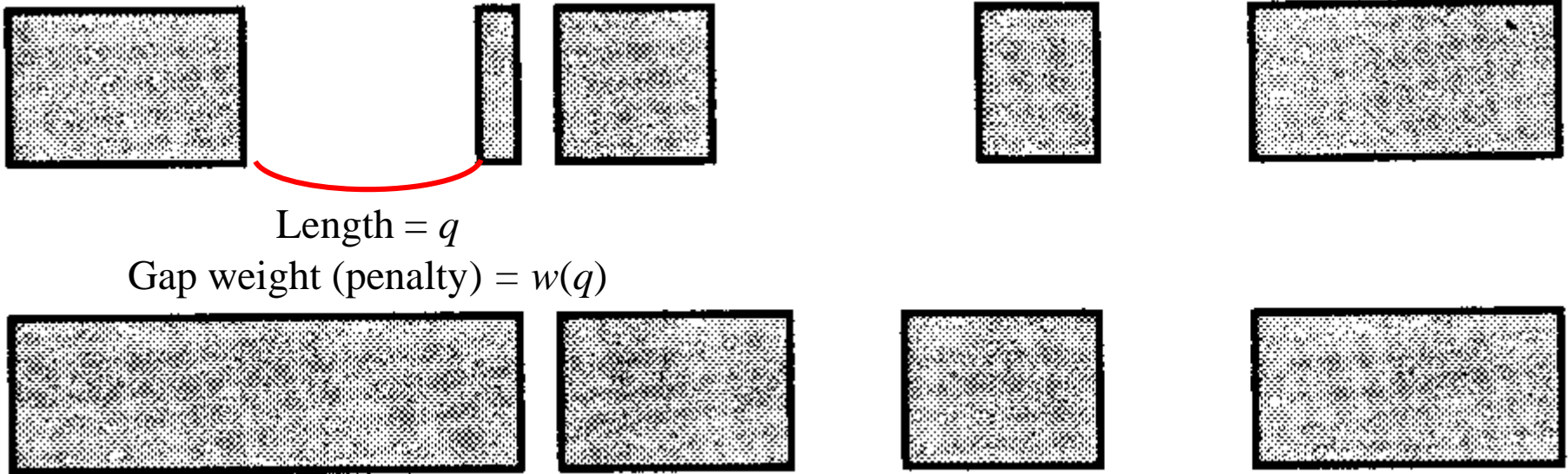
2014. 10. 21

ISA Lab

배준우

Gap weight

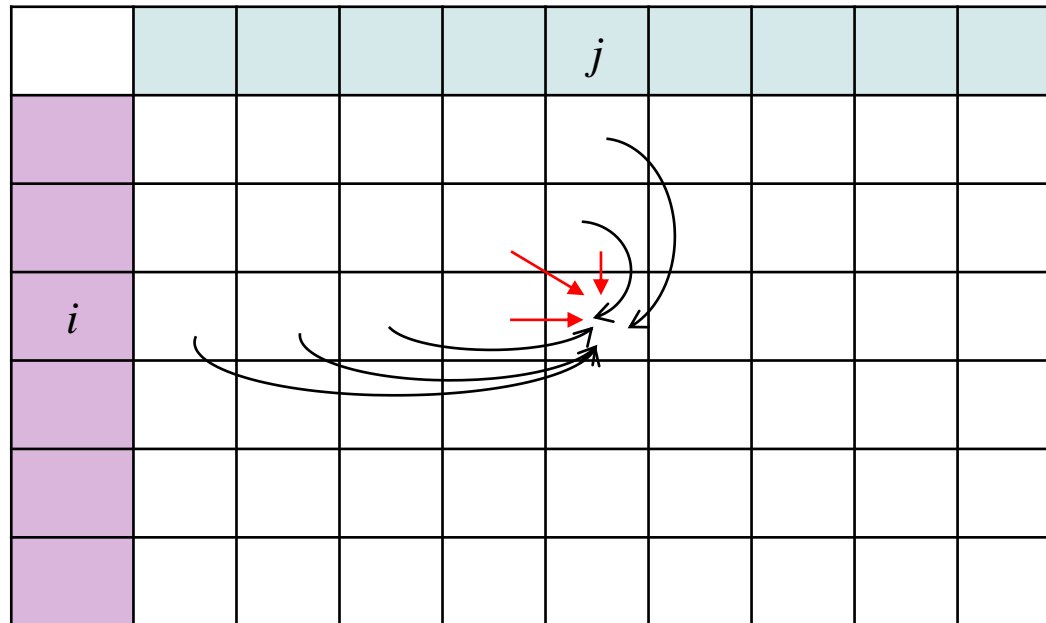
- Gap weight



Gap weight

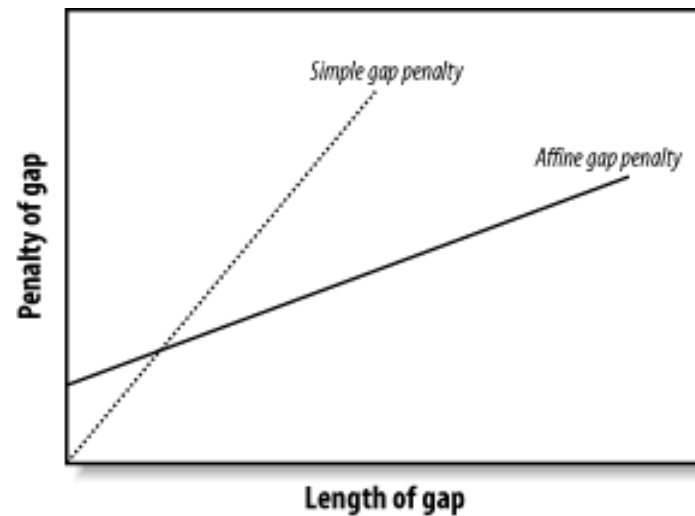
- **Arbitrary gap weight**

- Any gap weight function is acceptable (this is the most general case)
- Weight of a gap is an arbitrary function $w(q)$ of its length
- The constant, affine and convex weight models are of course subcases of the arbitrary weight model



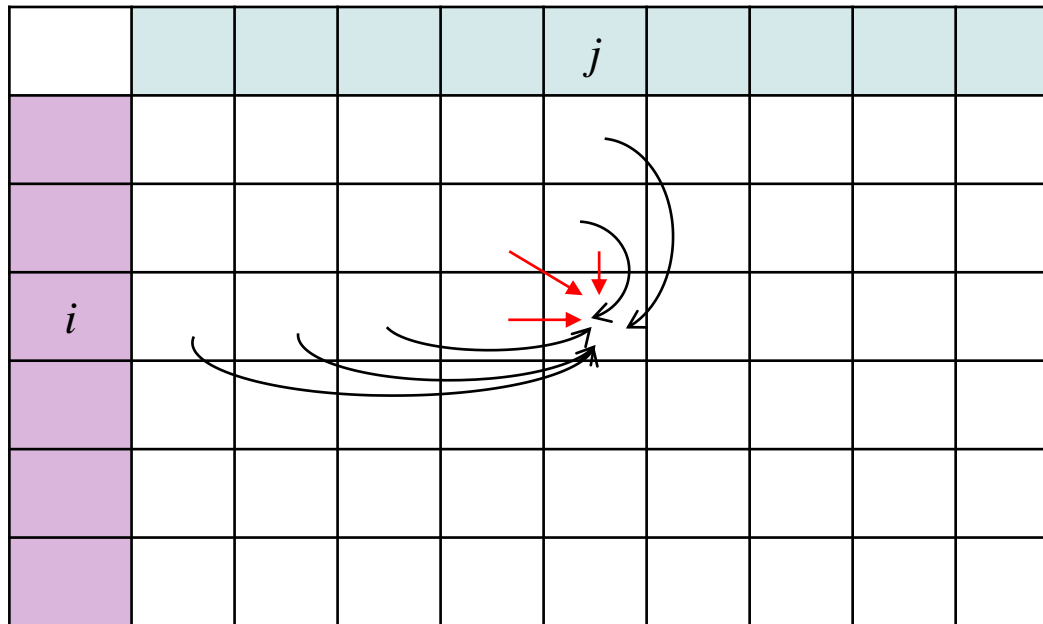
Gap weight

- **Affine gap weight**
 - The model most commonly used by molecular biologists



Gap weight

- **Affine gap weight**
 - The model most commonly used by molecular biologists



Gap weight

- **Convex gap weight**
 - More difficult to solve than with affine gap weights
 - Not as difficult as the problem with arbitrary gap weights

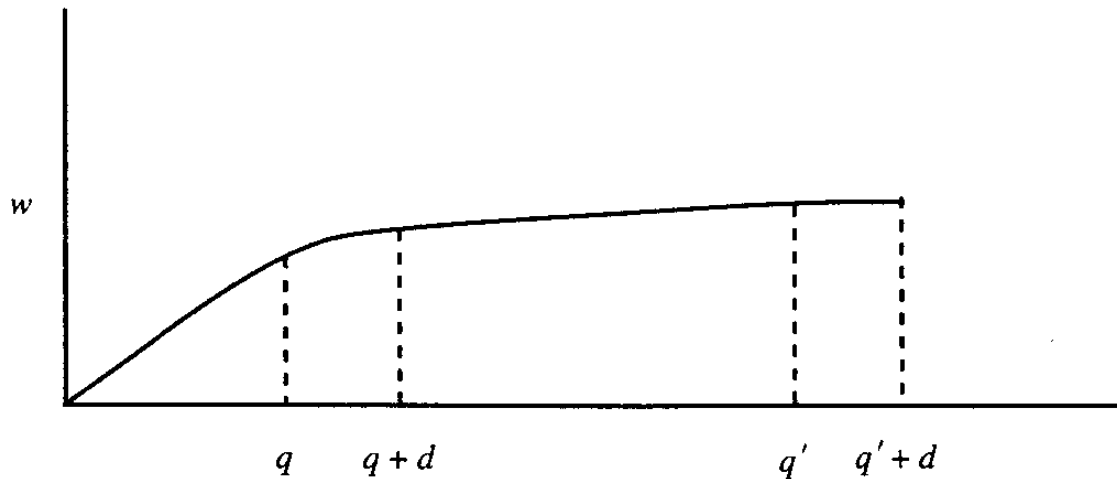


Figure 12.16: A convex function w .

Gap weight

- **Time complexity**
 - Arbitrary gap weights: $O(n^2m)$
 - Affine gap weights: $O(nm)$
 - Convex gap weights: $O(nm \log n)$
- Affine < Convex < Arbitrary
- We will discuss convex gap weights in terms of similarity
 - maximum weighted alignment

Convex gap weight

- **Definition**

- Assume that $w(q)$ is a nonnegative function of length q .
- Then $w(q)$ is **convex** if and only if $w(q+1) - w(q) \leq w(q) - w(q-1)$ for every q .
- It follows that $w(q+d) - w(q) \geq w(q'+d) - w(q')$ for $q < q'$ for any fixed d .

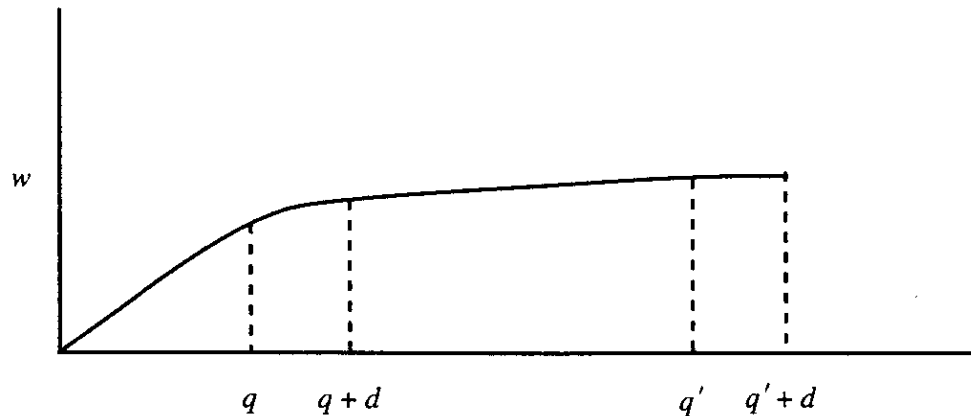
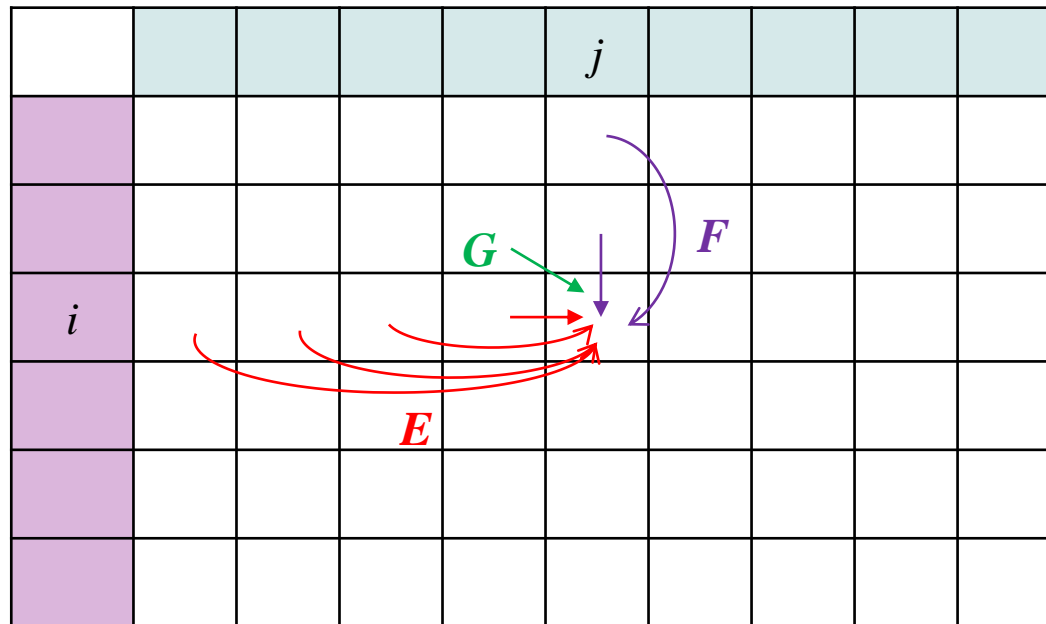


Figure 12.16: A convex function w .

Convex gap weight

- **Speeding up the general recurrences**
 - use the same dynamic programming recurrences developed for arbitrary gap weights
 - but reduce the time needed to evaluate those recurrences



Convex gap weight

- **Speeding up the general recurrences**
 - use the same dynamic programming recurrences developed for arbitrary gap weights
 - but reduce the time needed to evaluate those recurrences

$$\begin{aligned} V(i, j) &= \max[E(i, j), F(i, j), G(i, j)], \\ G(i, j) &= V(i-1, j-1) + s(S_1(i), S_2(j)), \\ E(i, j) &= \max_{0 \leq k \leq j-1} [V(i, k) - w(j-k)], \\ F(i, j) &= \max_{0 \leq l \leq i-1} [V(l, j) - w(i-l)], \\ V(i, 0) &= -w(i), \\ V(0, j) &= -w(j), \\ E(i, 0) &= -w(i), \\ F(0, j) &= -w(j). \end{aligned}$$

$O(n)$ per row

$O(n^2)$ per row

$O(m^2)$ per column

Convex gap weight

- Simplifying notation

$$E(i, j) = \max_{0 \leq k \leq j-1} [V(i, k) - w(j - k)]$$



In any fixed row, we can drop the row index i

$$E(j) = \max_{0 \leq k \leq j-1} [V(k) - w(j - k)]$$

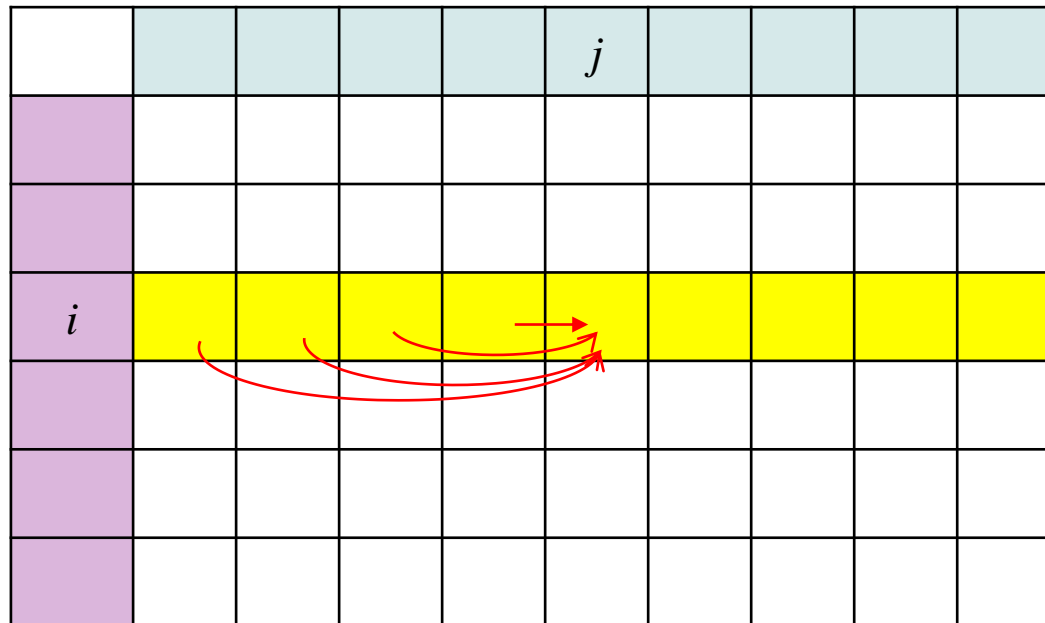


$$Cand(k, j) = V(k) - w(j - k)$$

$$E(j) = \max_{0 \leq k \leq j-1} Cand(k, j)$$

Convex gap weight

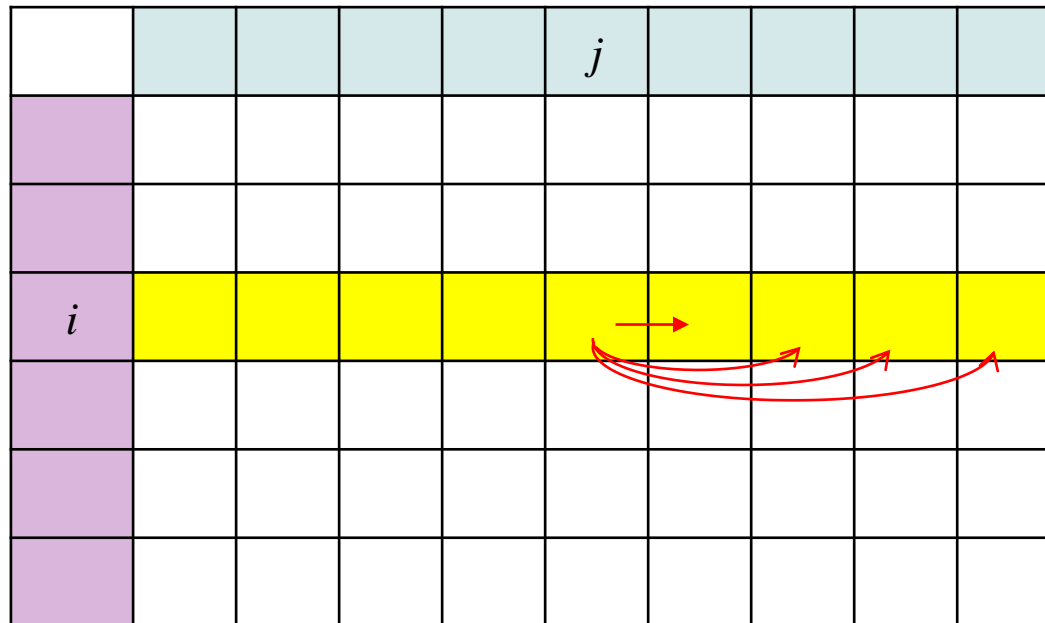
- **Forward dynamic programming**
 - It is more helpful in this exposition



Backward dynamic programming

Convex gap weight

- **Forward dynamic programming**
 - It is more helpful in this exposition



Forward dynamic programming

Convex gap weight

- Forward dynamic programming

$\bar{E}(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n

$E(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n

Convex gap weight

- Forward dynamic programming

$\bar{E}(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$Cand(0,1)$	$Cand(0,2)$...	$Cand(0,j-1)$	$Cand(0,j)$	$Cand(0,j+1)$...	$Cand(0,n-1)$	$Cand(0,n)$

$E(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n

Convex gap weight

- Forward dynamic programming

$\bar{E}(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$Cand(0,1)$	$Cand(0,2)$...	$Cand(0,j-1)$	$Cand(0,j)$	$Cand(0,j+1)$...	$Cand(0,n-1)$	$Cand(0,n)$

$E(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$\bar{E}(1)$								

Convex gap weight

- Forward dynamic programming

$\bar{E}(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$Cand(0,1)$	$Cand(0,2)$...	$Cand(0,j-1)$	$Cand(0,j)$	$Cand(0,j+1)$...	$Cand(0,n-1)$	$Cand(0,n)$

$Cand(1,2)$...	$Cand(1,j-1)$	$Cand(1,j)$	$Cand(1,j+1)$...	$Cand(1,n-1)$	$Cand(1,n)$
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Assume $>$

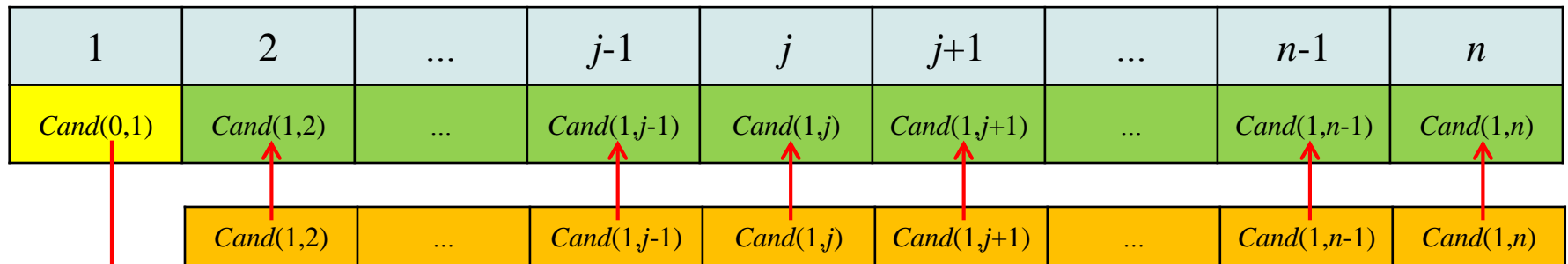
$E(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$\bar{E}(1)$								

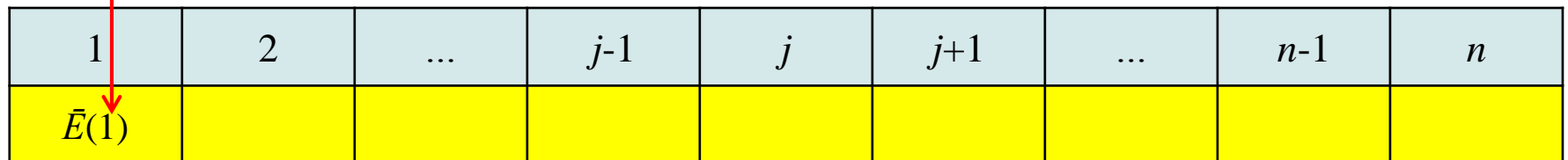
Convex gap weight

- Forward dynamic programming

$\bar{E}(j)$



$E(j)$



Convex gap weight

- Forward dynamic programming

$\bar{E}(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$Cand(0,1)$	$Cand(1,2)$...	$Cand(1,j-1)$	$Cand(1,j)$	$Cand(1,j+1)$...	$Cand(1,n-1)$	$Cand(1,n)$

...	$Cand(2,j-1)$	$Cand(2,j)$	$Cand(2,j+1)$...	$Cand(2,n-1)$	$Cand(2,n)$
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$E(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$\bar{E}(1)$	$\bar{E}(2)$							

Convex gap weight

Forward dynamic programming for a fixed row

```
For  $j := 1$  to  $m$  do  
begin  
 $\bar{E}(j) := \text{Cand}(0, j)$ ;  
end;
```

initialize

```
For  $j := 1$  to  $m$  do  
begin  
 $E(j) := \bar{E}(j)$ ;  
 $V(j) := \max[G(j), E(j), F(j)]$ ;  
{We assume, but do not show that  $F(j)$  and  $G(j)$   
have been computed for cell  $j$  in the row.}
```

Set $E(j)$ to the current $\bar{E}(j)$

```
For  $j' := j + 1$  to  $m$  do {Loop 1}  
  if  $\bar{E}(j') < \text{Cand}(j, j')$  then  
    begin  
       $\bar{E}(j') := \text{Cand}(j, j')$ ;  
    end
```

Traverse forwards to set $\bar{E}(j')$

```
end;
```

Convex gap weight

- **Forward dynamic programming**
 - An alternative way to think about forward dynamic programming
 - >Weighted edit graph for alignment problem
 - Optimal distances = optimal alignments
 - Distance algorithms(such as Dijkstra's algorithm) for shortest distance can be described as forward looking

Convex gap weight

- **Forward dynamic programming**
 - Time complexity
 - Both backward and forward dynamic programming
 - Exactly the same arithmetic operations and comparisons are done
 - Still requires $\Theta(n^2)$ time per row
 - No faster than backwards dynamic programming

Convex gap weight

- The basis of the speedup

$\bar{E}(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$Cand(0,1)$	$Cand(1,2)$...	$Cand(5,j-1)$	$Cand(j-1,j)$	$Cand(j-1,j+1)$...	$Cand(j-1,n-1)$	$Cand(j-1,n)$

$Cand(j,j+1)$...	$Cand(j,n-1)$	$Cand(j,n)$
---------------	-----	---------------	-------------

If > \leadsto **Win**
 else \leadsto **lose**

$E(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$\bar{E}(1)$	$\bar{E}(2)$...	$\bar{E}(j-1)$	$\bar{E}(j)$				

Convex gap weight

- **The basis of the speedup**
 - *Candidate list* approach
 - The speedup works
 - by identifying and eliminating large numbers of candidate values
 - that have **no chance of winning any comparison**
 - Key observation
 - Let j be the current cell.
 - If $Cand(j, j') \leq \bar{E}(j')$ for some $j' > j$,
 - then $Cand(j, j'') \leq \bar{E}(j'')$ for every $j'' > j'$

Convex gap weight

- The basis of the speedup

$\bar{E}(j)$

1	...	$j-1$	j	$j+1$	$j+2$...	$n-1$	n
$\bar{E}(1)$...	$\bar{E}(j-1)$	$\bar{E}(j)$	$\bar{E}(j+1)$	$\bar{E}(j+2)$...	$\bar{E}(n-1)$	$\bar{E}(n)$


$Cand(j,j+1)$

$Cand(j,j+2)$

...

$Cand(j,n-1)$

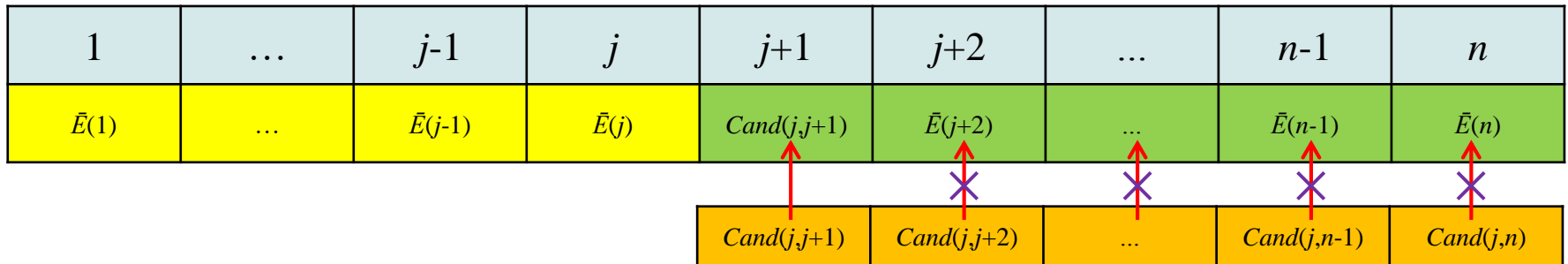
$Cand(j,n)$



Convex gap weight

- The basis of the speedup

$\bar{E}(j)$



Convex gap weight

- The basis of the speedup
 - Lemma 12.6.1
 - Let $k < j < j' < j''$ be any four cells in the same row.
 - If $Cand(j, j') \leq Cand(k, j')$ then $Cand(j, j'') \leq Cand(k, j'')$

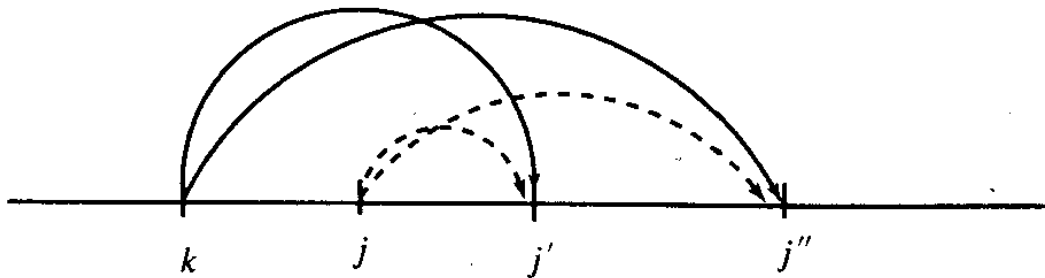


Figure 12.17: Graphical illustration of the *key observation*. Winning candidates are shown with a solid curve and losers with a dashed curve. If the candidate from j loses to the candidate from k at cell j' , then the candidate from j will lose to the candidate from k at every cell j'' to the right of j' .

Convex gap weight

- The basis of the speedup

- Lemma 12.6.1

- Let $k < j < j' < j''$ be any four cells in the same row.
 - If $Cand(j, j') \leq Cand(k, j')$ then $Cand(j, j'') \leq Cand(k, j'')$

- PROOF

- $Cand(k, j) = V(k) - w(j - k)$

$$\begin{aligned} V(k) - w(j' - k) &\geq V(j) - w(j' - j) \\ V(k) - V(j) &\geq w(j' - k) - w(j' - j) \end{aligned}$$

Convex gap weight

- The basis of the speedup

- Lemma 12.6.1

- Let $k < j < j' < j''$ be any four cells in the same row.
- If $\text{Cand}(j, j') \leq \text{Cand}(k, j')$ then $\text{Cand}(j, j'') \leq \text{Cand}(k, j'')$

- PROOF

- $\text{Cand}(k, j) = V(k) - w(j - k)$

$$\begin{aligned} V(k) - w(j' - k) &\geq V(j) - w(j' - j) \\ V(k) - V(j) &\geq w(j' - k) - w(j' - j) \end{aligned}$$

- By convexity, $w(j' - k) - w(j' - j) \geq w(j'' - k) - w(j'' - j)$
- $V(k) - V(j) \geq w(j'' - k) - w(j'' - j)$
- $V(k) - w(j'' - k) \geq V(j) - w(j'' - j)$

Convex gap weight

- The basis of the speedup

- Lemma 12.6.1

- Let $k < j < j' < j''$ be any four cells in the same row.
 - If $\text{Cand}(j, j') \leq \text{Cand}(k, j')$ then $\text{Cand}(j, j'') \leq \text{Cand}(k, j'')$ ←

- PROOF

- $\text{Cand}(k, j) = V(k) - w(j - k)$

$$\begin{aligned} V(k) - w(j' - k) &\geq V(j) - w(j' - j) \\ V(k) - V(j) &\geq w(j' - k) - w(j' - j) \end{aligned}$$

- By convexity, $w(j' - k) - w(j' - j) \geq w(j'' - k) - w(j'' - j)$
 - $V(k) - V(j) \geq w(j'' - k) - w(j'' - j)$
 - $V(k) - w(j'' - k) \geq V(j) - w(j'' - j)$

Convex gap weight

- The basis of the speedup

Forward dynamic programming for a fixed row

For $j := 1$ to m do

begin

$\bar{E}(j) := \text{Cand}(0, j);$

end;

For $j := 1$ to m do

begin

$E(j) := \bar{E}(j);$

$V(j) := \max[G(j), E(j), F(j)];$

{We assume, but do not show that $F(j)$ and $G(j)$
have been computed for cell j in the row.}

But this improvement does not lead
directly to a better (worst-case) time
bound

For $j' := j + 1$ to m do {Loop 1}

if $\bar{E}(j') < \text{Cand}(j, j')$ then

begin

$\bar{E}(j') := \text{Cand}(j, j');$

end

else then
break

end;

Convex gap weight

- Cell pointers and row partition

Forward dynamic programming for a fixed row

For $j := 1$ to m do

begin

$\bar{E}(j) := \text{Cand}(0, j);$

$b(j) := 0$

end;

For $j := 1$ to m do

begin

$E(j) := \bar{E}(j);$

$V(j) := \max[G(j), E(j), F(j)];$

{We assume, but do not show that $F(j)$ and $G(j)$
have been computed for cell j in the row.}

For $j' := j + 1$ to m do {Loop 1}

if $\bar{E}(j') < \text{Cand}(j, j')$ then

begin

$\bar{E}(j') := \text{Cand}(j, j');$

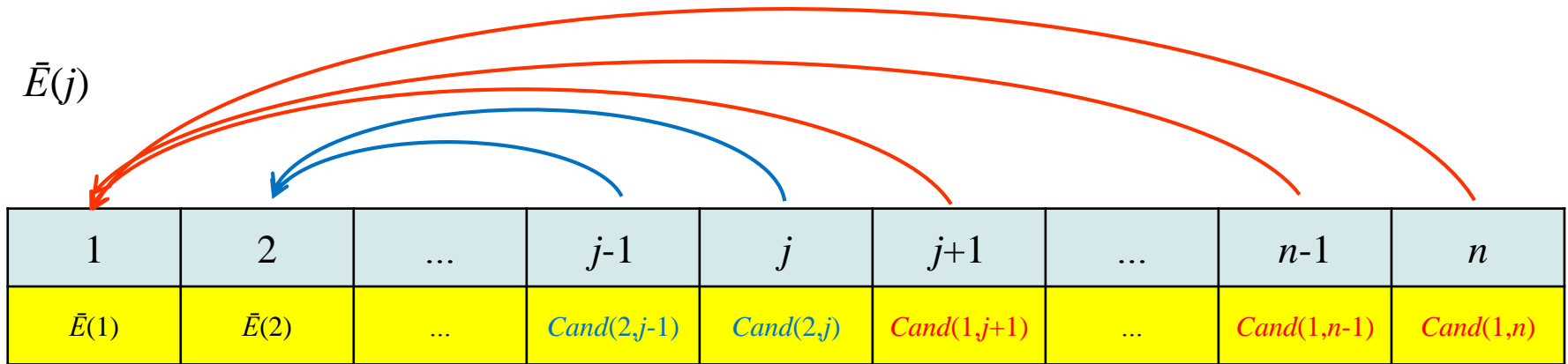
$b(j') := j$; {This sets a pointer from j' to j to be explained later.}

end

end;

Convex gap weight

- Cell pointers and row partition

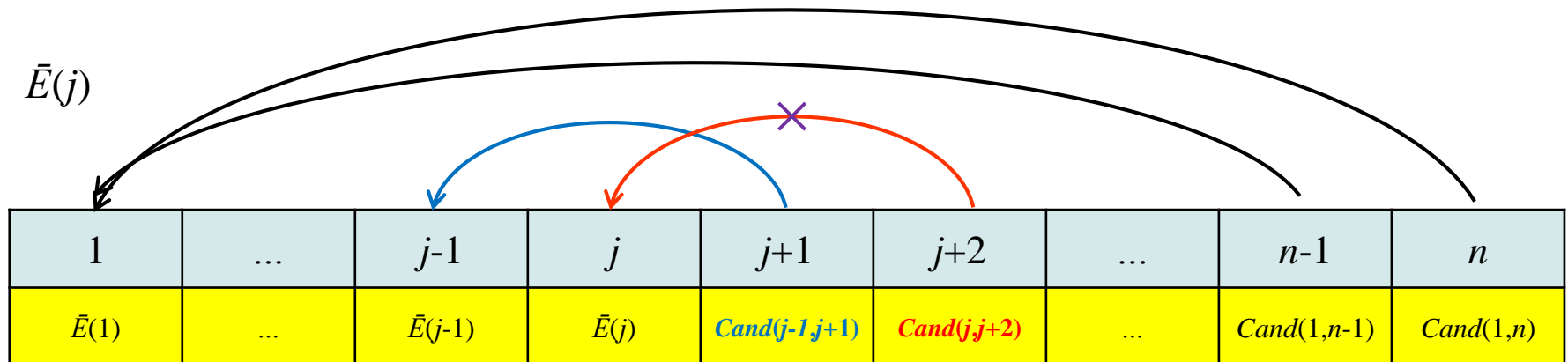


Convex gap weight

- **Cell pointers and row partition**

- Lemma 12.6.2

- Consider the point when j is the current cell
- but before j sends forward any candidate values
- At that point, $b(j') \geq b(j'+1)$ for every cell j' from $j+1$ to $m-1$



Convex gap weight

- **Cell pointers and row partition**
 - Lemma 12.6.2
 - Consider the point when j is the current cell
 - but before j sends forward any candidate values
 - At that point, $b(j') \geq b(j'+1)$ for every cell j' from $j+1$ to $m-1$
 - PROOF
 - Suppose $b(j') < b(j'+1)$
 - By Lemma 12.6.1, $Cand(b(j'), j'+1) \geq Cand(b(j'+1), j'+1)$
 - $b(j'+1)$ should be set to $b(j')$, not $b(j'+1)$
 - Hence $b(j') \geq b(j'+1)$

Convex gap weight

- **Cell pointers and row partition**

- Corollary 12.6.1

- j is the current cell, but before j sends forward any candidates
- The values of the b pointers form a **nonincreasing** sequence from left to right
- Therefore, cells $j, j+1, j+2, \dots, m$ are **partitioned into maximal blocks** of consecutive cells
 - such that all b pointers in the block have the same value
 - and the pointer values decline in successive blocks

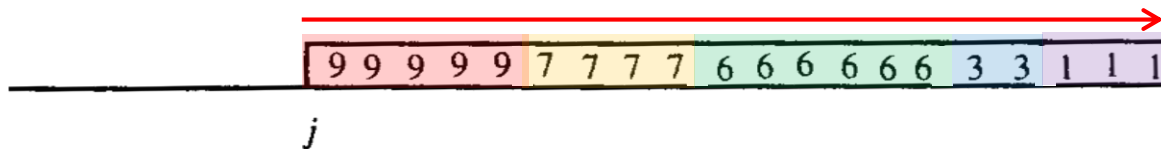


Figure 12.18: Partition of the cells $j + 1$ through m into maximal blocks of consecutive cells such that all the cells in any block have the same b value. The common b value in any block is less than the common b value in the preceding block.

Convex gap weight

- **Cell pointers and row partition**
 - Given Corollary 12.6.1
 - The algorithm doesn't need to explicitly maintain a b pointer for every cell
 - Only record the **common b pointer** for each block

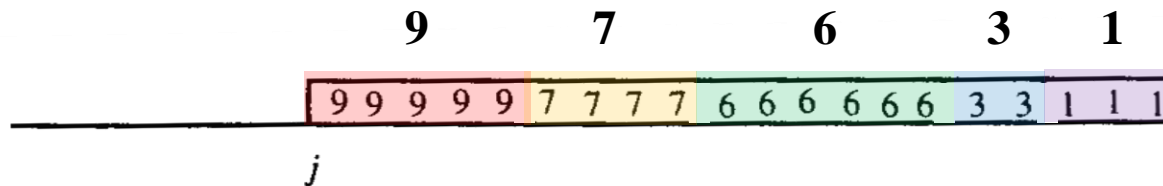


Figure 12.18: Partition of the cells $j + 1$ through m into maximal blocks of consecutive cells such that all the cells in any block have the same b value. The common b value in any block is less than the common b value in the preceding block.

Convex gap weight

- **Preparation for the speedup**
 - Our goal
 - To reduce the time per row used in computing the E values
 - $\Theta(n^2) \rightarrow O(n \log n)$
 - The main work done in a row
 1. Update the \bar{E} values
 2. Update the current block-partition with its associated pointer

Convex gap weight

- **Preparation for the speedup**
 - Our goal
 - To reduce the time per row used in computing the E values
 - $\Theta(n^2) \rightarrow O(n \log n)$
 - The main work done in a row
 1. Update the \bar{E} values
 - Assume that all the \bar{E} values are maintained for free
 2. **Update the current block-partition** with its associated pointer

Convex gap weight

- Preparation for the speedup

$\bar{E}(j)$

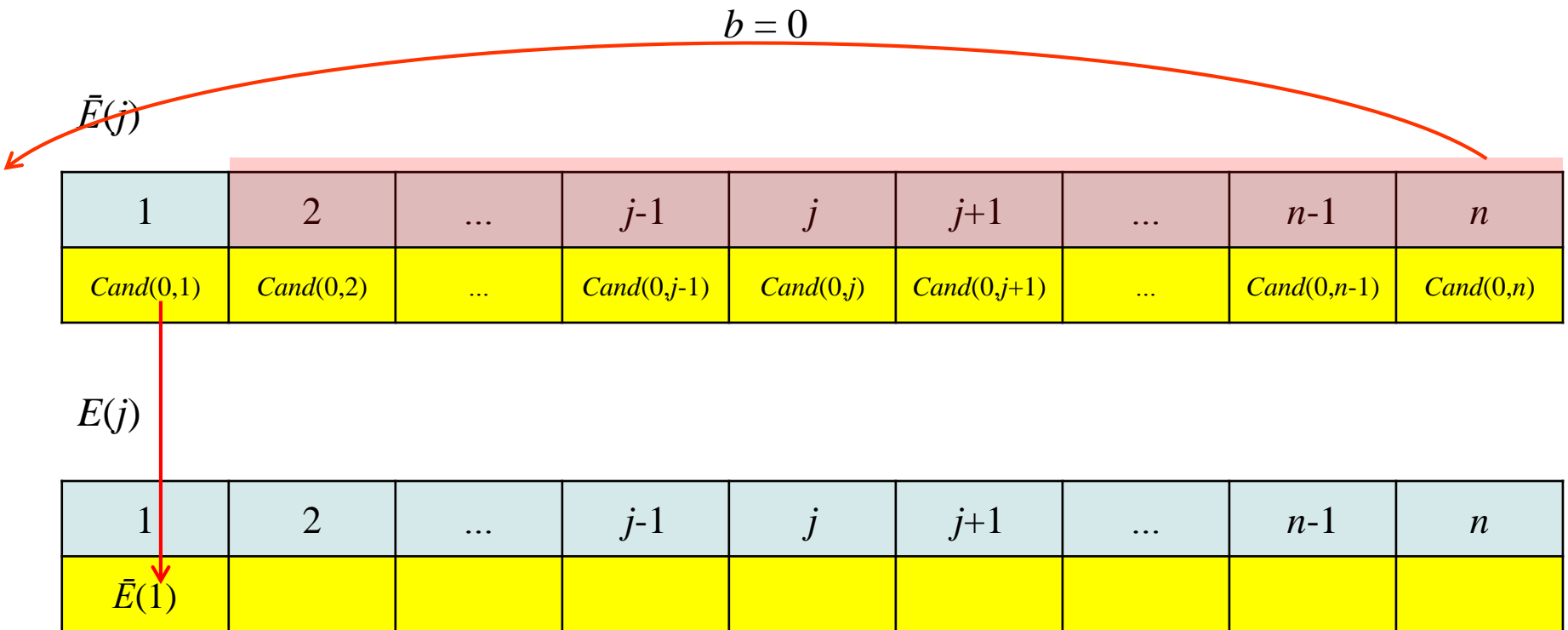
1	2	...	$j-1$	j	$j+1$...	$n-1$	n
$Cand(0,1)$	$Cand(0,2)$...	$Cand(0,j-1)$	$Cand(0,j)$	$Cand(0,j+1)$...	$Cand(0,n-1)$	$Cand(0,n)$

$E(j)$

1	2	...	$j-1$	j	$j+1$...	$n-1$	n

Convex gap weight

- Preparation for the speedup

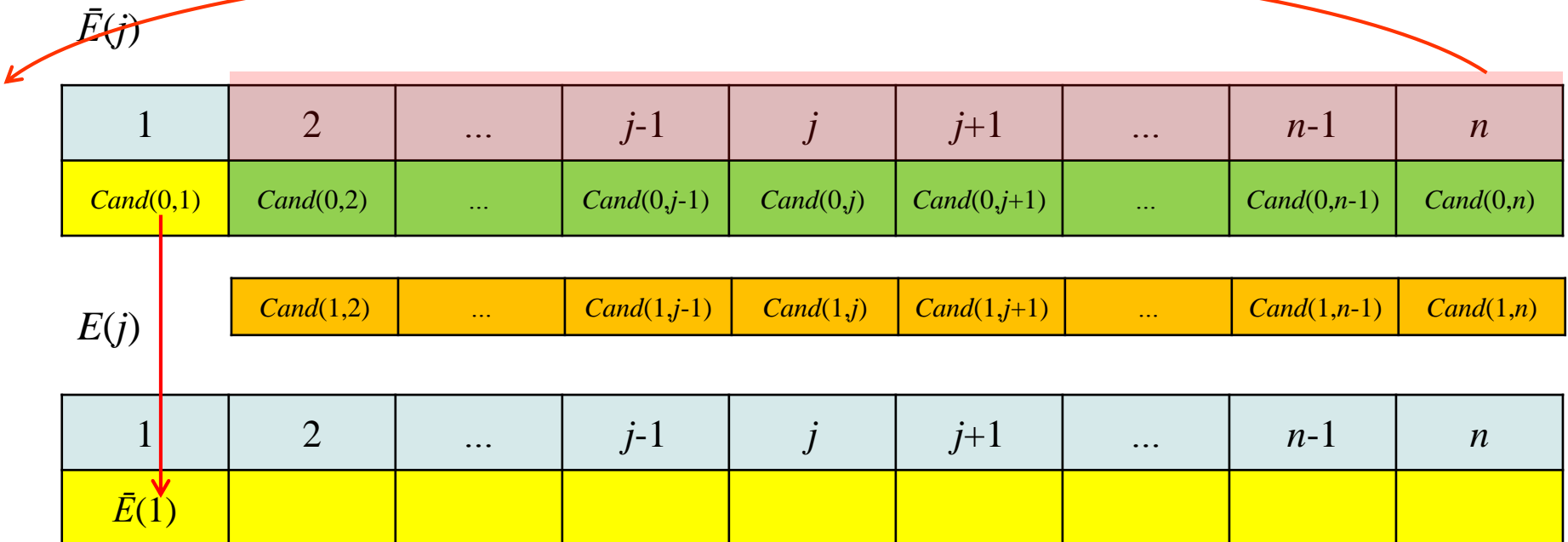


Convex gap weight

- Preparation for the speedup

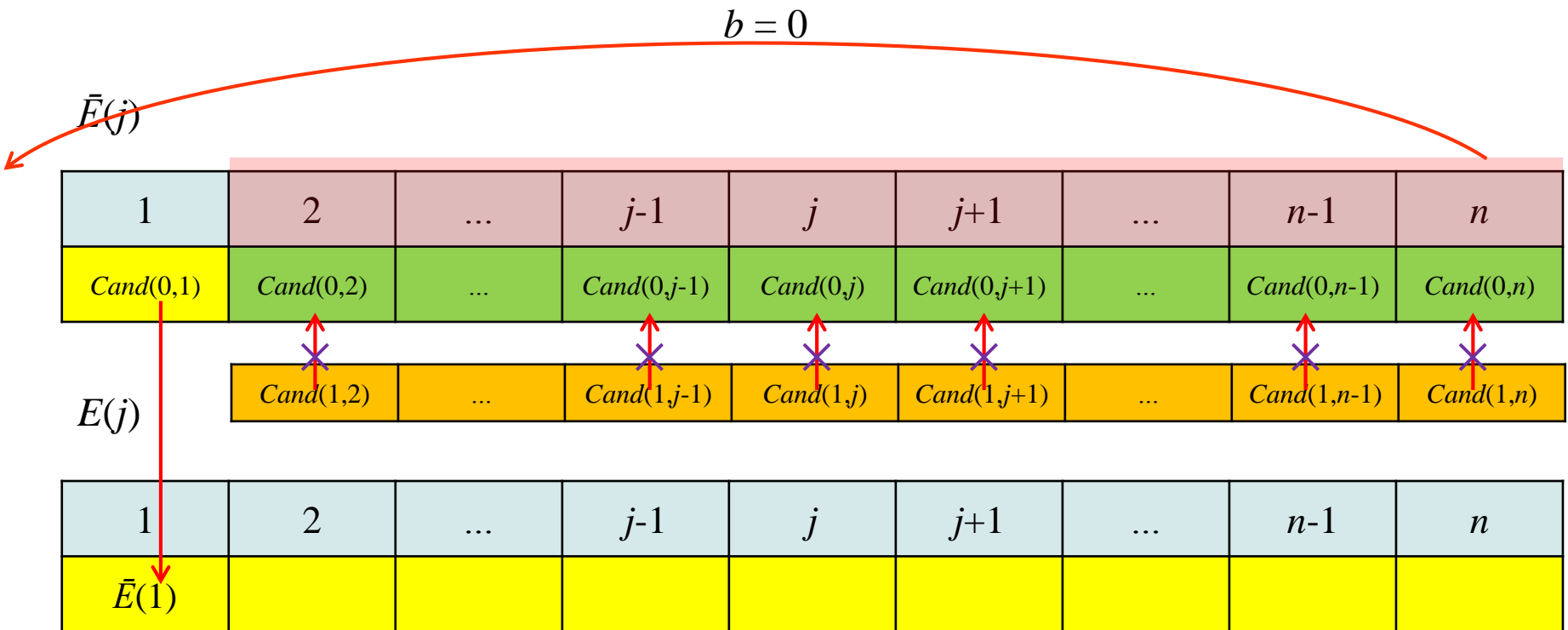
There are only **three cases** for the new block-partition

$b = 0$



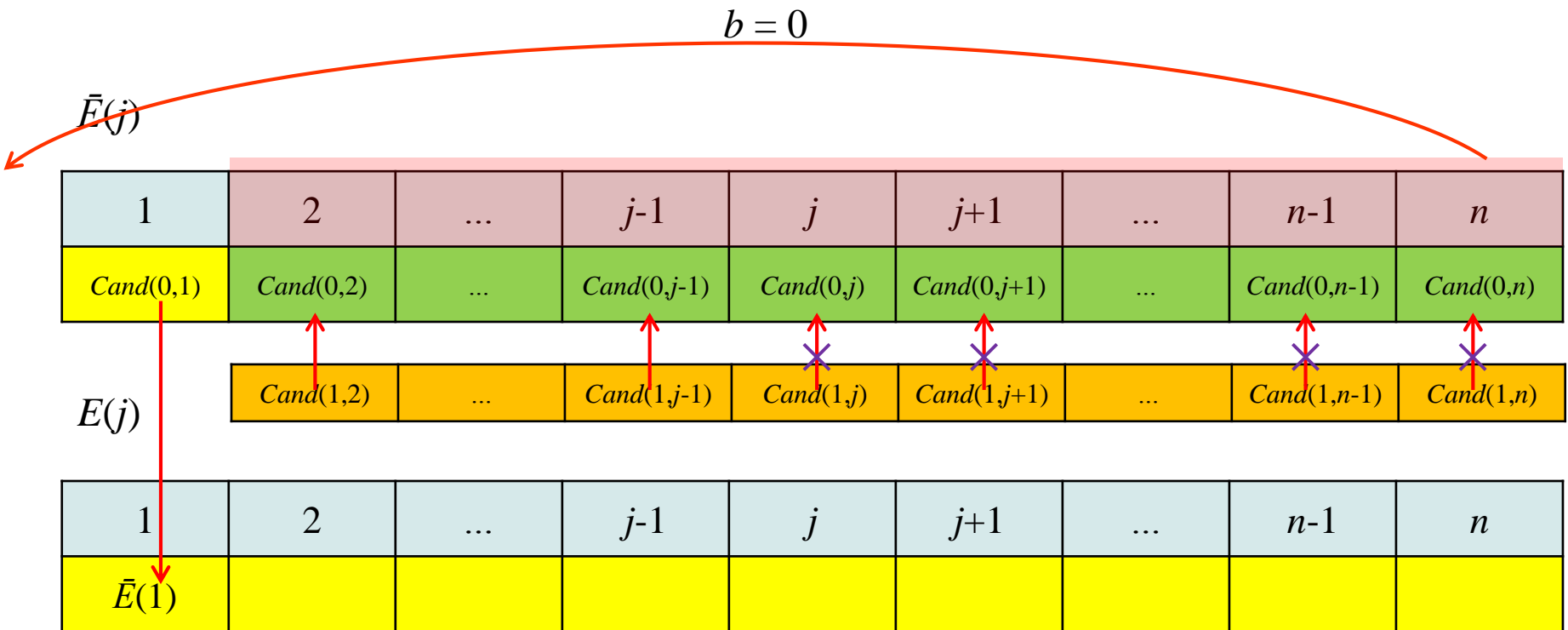
Convex gap weight

- **Preparation for the speedup**
 - Case 1: remain in a **single block** with common pointer $b = 0$



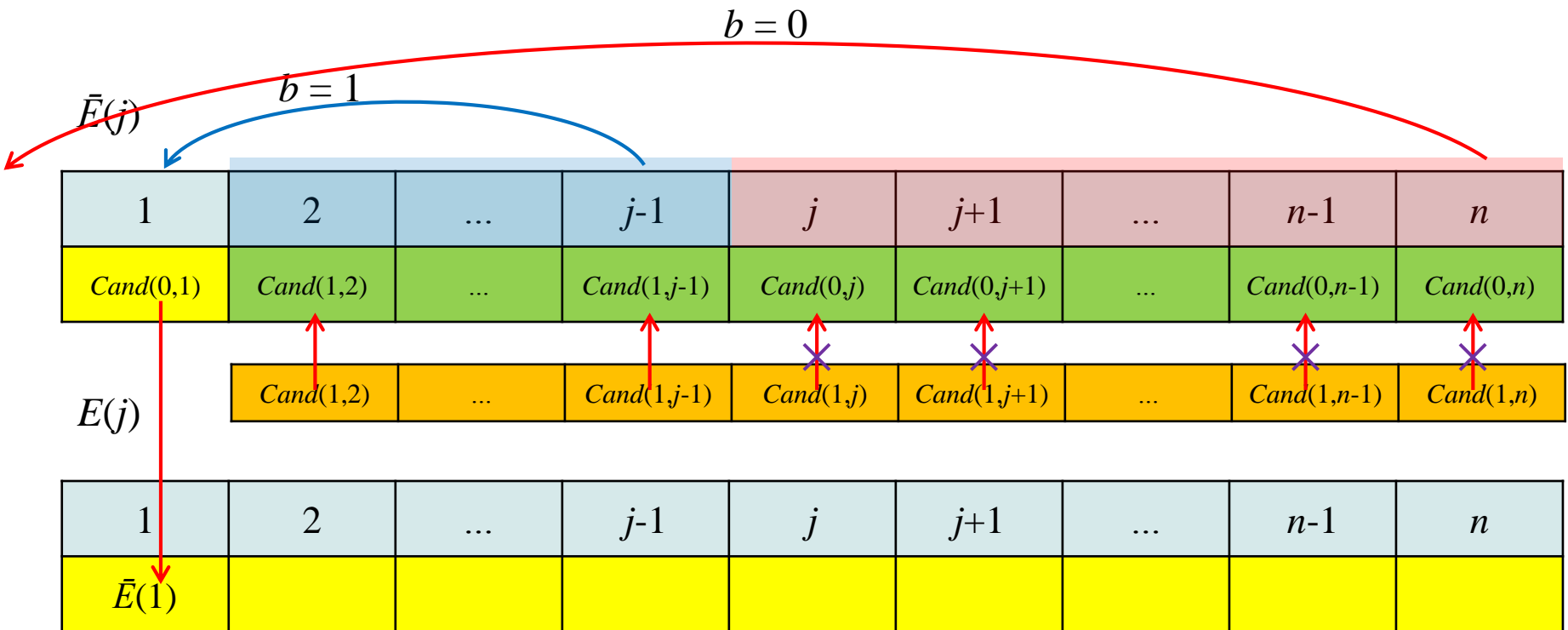
Convex gap weight

- **Preparation for the speedup**
 - Case 2: divided into **two blocks**



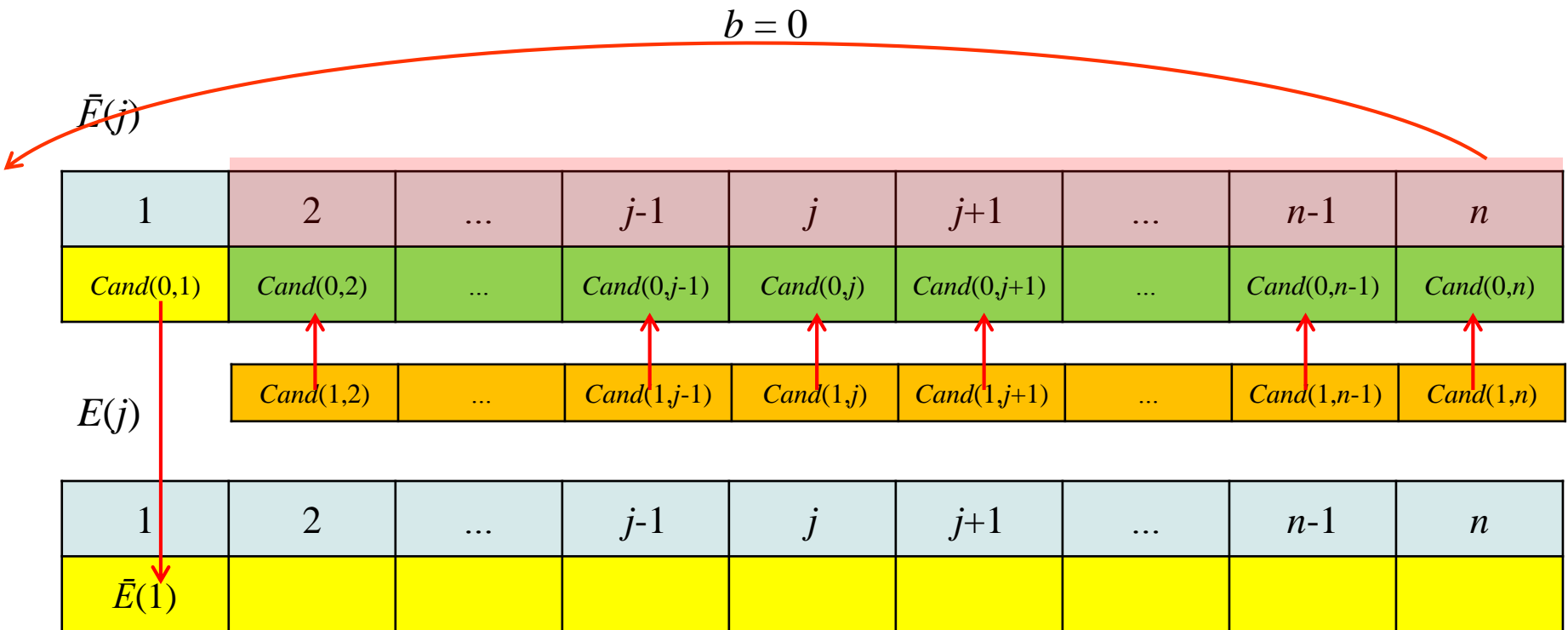
Convex gap weight

- **Preparation for the speedup**
 - Case 2: divided into **two blocks**



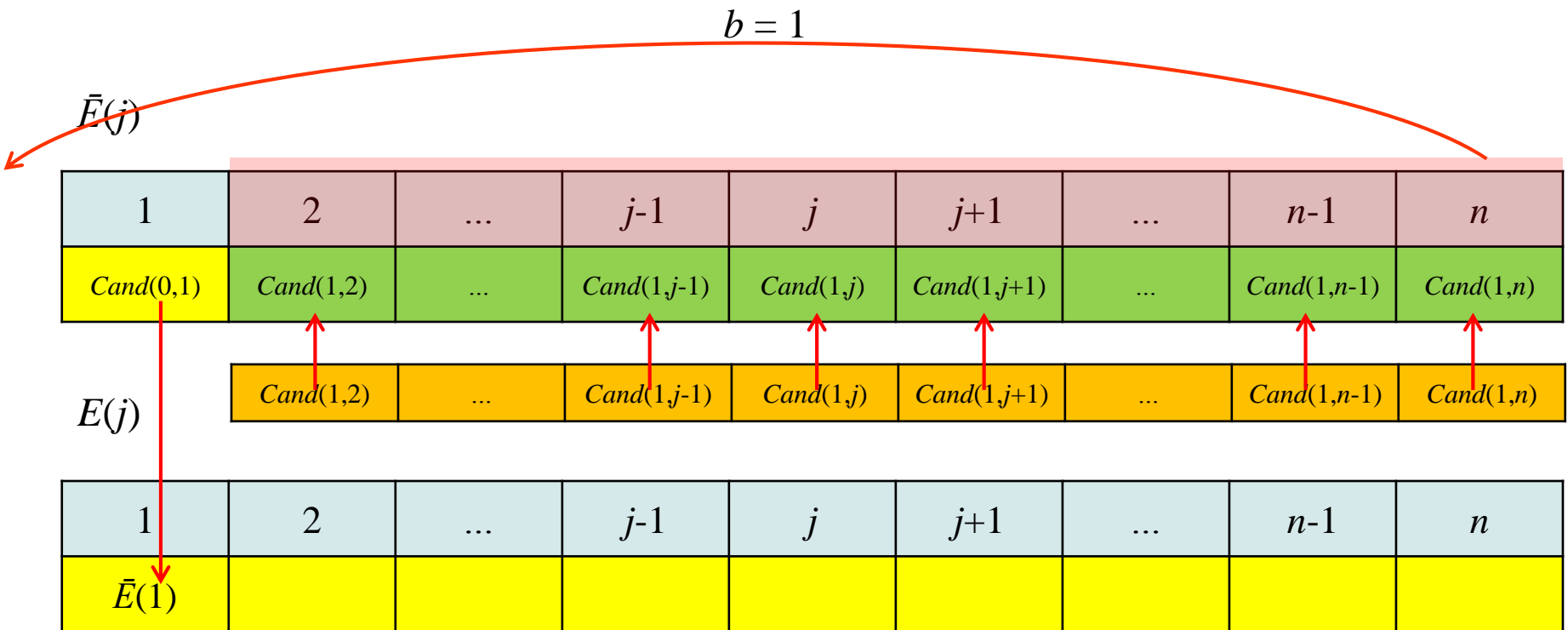
Convex gap weight

- **Preparation for the speedup**
 - Case 3: remain in a **single block** with common pointer $b = 1$



Convex gap weight

- **Preparation for the speedup**
 - Case 3: remain in a **single block** with common pointer $b = 1$

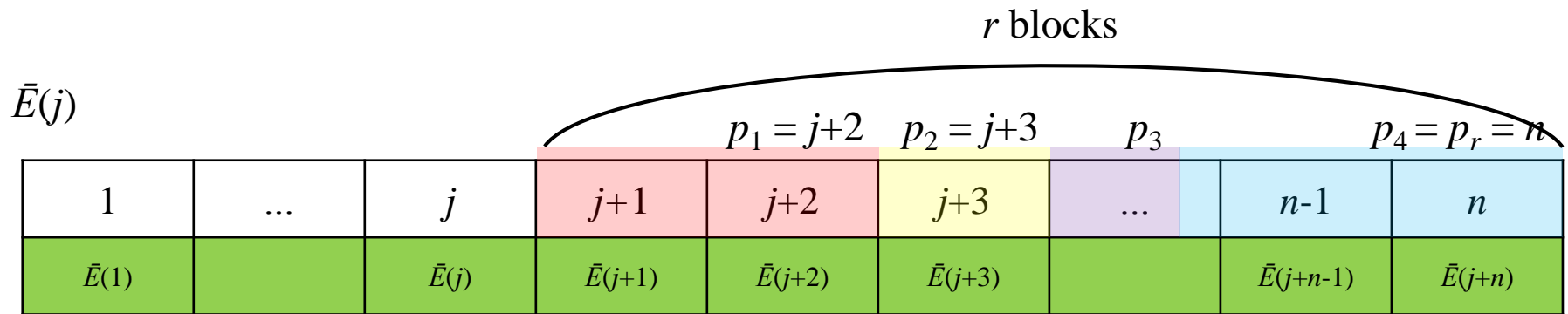


Convex gap weight

- **Preparation for the speedup**
 - The punch line
 - Search for the left-most cell $j' > 2$ such that $\bar{E}(j') \geq Cand(1, j')$
 - *Win ... Win **Lose** Lose ... Lose*
 - can be done by **binary search**
 - $O(\log n)$ comparisons
 - at most one pointer update
 - Since we only record one b pointer per block

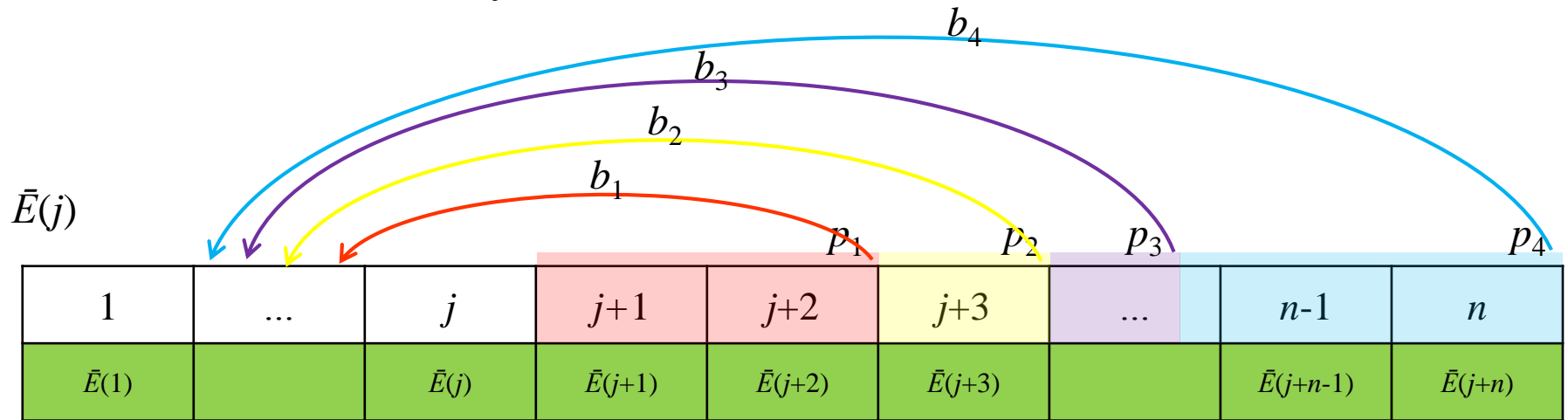
Convex gap weight

- **Preparation for the speedup**
 - General case of $j > 1$



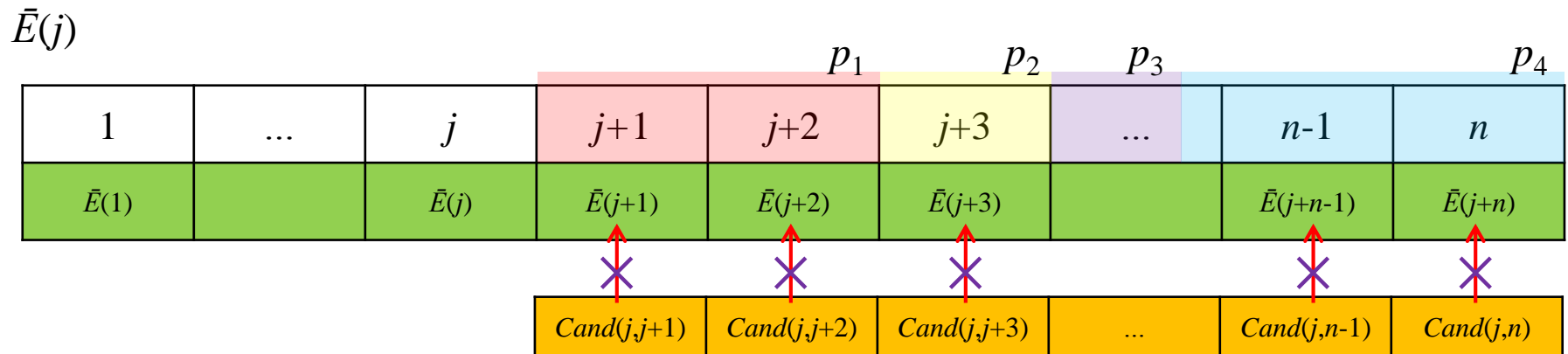
Convex gap weight

- **Preparation for the speedup**
 - General case of $j > 1$



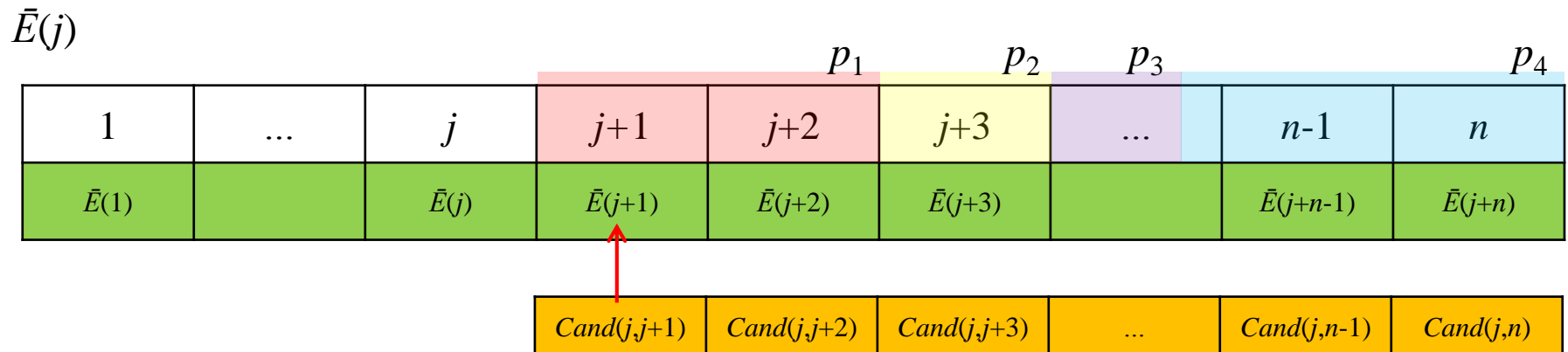
Convex gap weight

- **Preparation for the speedup**
 - Case 1: if $\bar{E}(j+1) \geq \text{Cand}(j, j+1)$ *Lose*



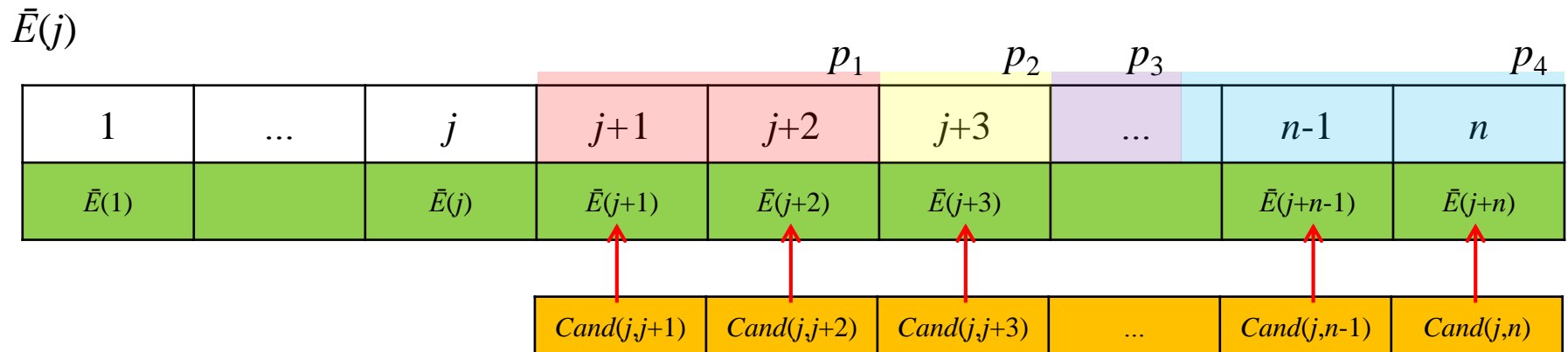
Convex gap weight

- **Preparation for the speedup**
 - Case 2: if $\bar{E}(j+1) < Cand(j, j+1)$ **Win**
 - until end-of-block list is exhausted
 - until it finds the first index s with $\bar{E}(p_s) \geq Cand(j, p_s)$



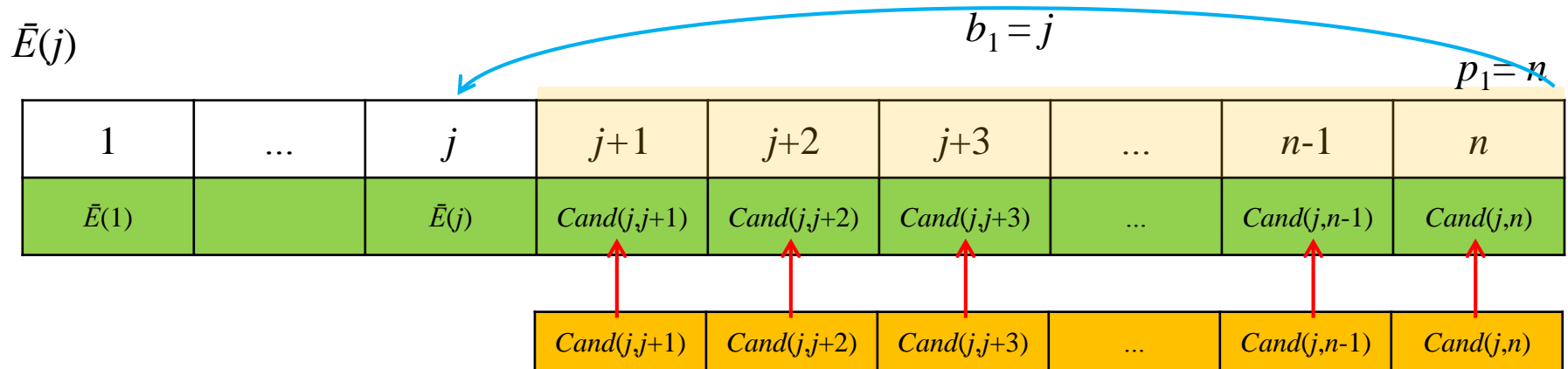
Convex gap weight

- **Preparation for the speedup**
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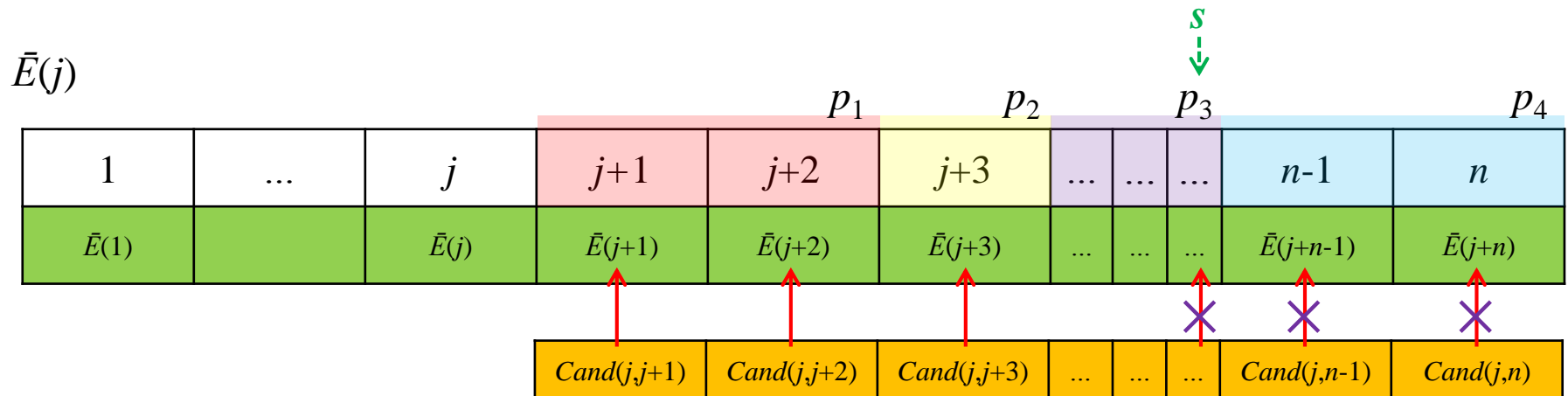
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- **Preparation for the speedup**
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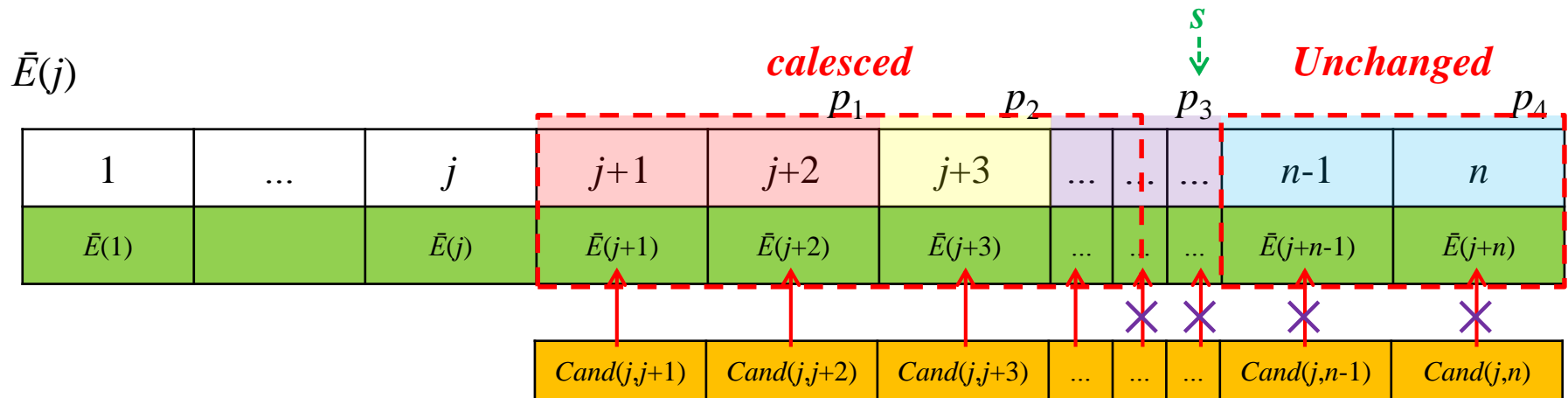
Convex gap weight

- **Preparation for the speedup**
 - Case 2: if $\bar{E}(j+1) < \text{Cand}(j, j+1)$ **Win**
 - A. until end-of-block list is exhausted
 - B. until it finds the first index s with $\bar{E}(p_s) \geq \text{Cand}(j, p_s)$



Convex gap weight

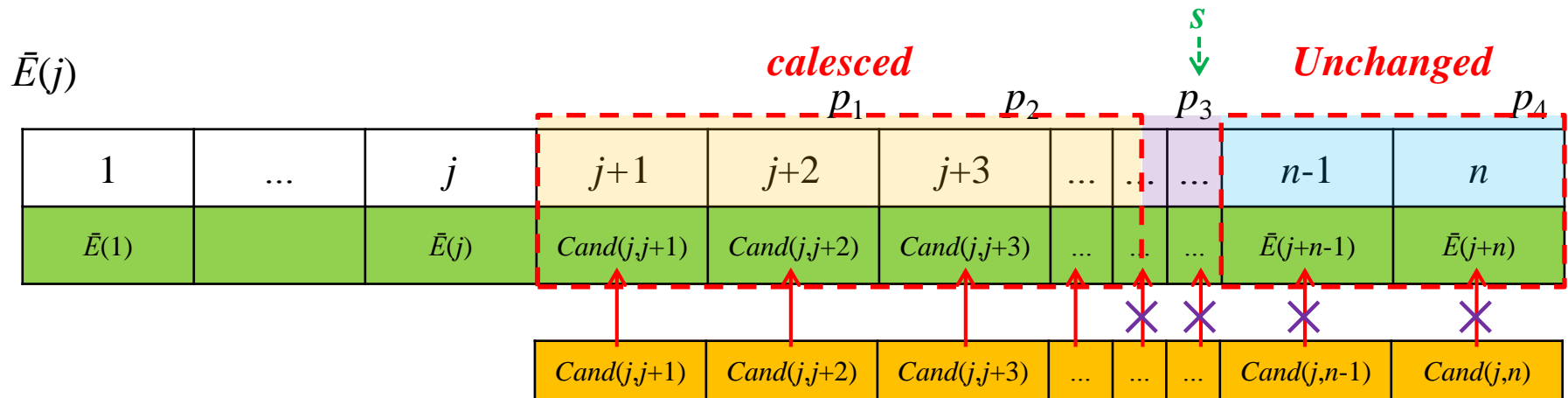
- **Preparation for the speedup**
 - Case 2: if $\bar{E}(j+1) < \text{Cand}(j, j+1)$ **Win**
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- The algorithm finds the proper place to split block s
 - by doing binary search over the cells in the block

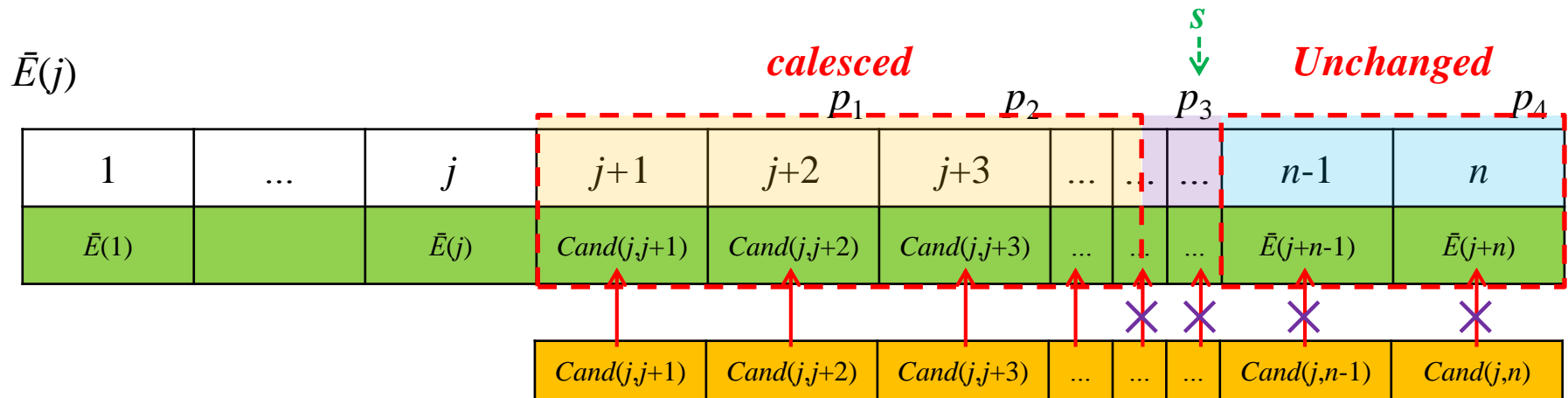
Convex gap weight

- **Preparation for the speedup**
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Convex gap weight

- **Preparation for the speedup**
 - Case 2: if $\bar{E}(j+1) < \text{Cand}(j, j+1)$ **Win**
 - until end-of-block list is exhausted
 - until it finds the first index s with $\bar{E}(p_s) \geq \text{Cand}(j, p_s)$



Convex gap weight

- **Final implementation details**
 - Our goal
 - To reduce the time per row used in computing the E values
 - $\Theta(n^2) \rightarrow O(n \log n)$
 - The main work done in a row
 1. **Update the \bar{E} values**
 - Assume that all the \bar{E} values are maintained for free
 2. Update the current block-partition with its associated pointer

Convex gap weight

- **Final implementation details**
 - The key observation
 - retrieves $\bar{E}(j)$
 - only when j is the current cell
 - retrieves $\bar{E}(j')$
 - only when examining cell j' in the process of updating the block-partition

Convex gap weight

- **Final implementation details**
 - The key observation
 - retrieves $\bar{E}(j)$
 - only when j is the current cell
 - j is always in the first block of the current block-partition
 - $b(j) = b_1$
 - $\bar{E}(j) = \text{Cand}(b_1, j)$
 - which can be computed in **constant time** when needed
 - retrieves $\bar{E}(j')$
 - only when examining cell j' in the process of updating the block-partition

Convex gap weight

- **Final implementation details**

- The key observation

- retrieves $\bar{E}(j)$

- only when j is the current cell
 - j is always in the first block of the current block-partition
 - $b(j) = b_1$
 - $\bar{E}(j) = \text{Cand}(b_1, j)$
 - which can be computed in **constant time** when needed

- retrieves $\bar{E}(j')$

- only when examining cell j' in the process of updating the block-partition
 - The algorithm knows the block that j' falls into, say block i ,
 - and hence it knows b_i
 - $\bar{E}(j') = \text{Cand}(b_i, j')$
 - which can be computed in **constant time** when needed

Convex gap weight

- **Final implementation details**

Revised forward dynamic programming for a fixed row

Initialize the end-of-block list to contain the single number m .

Initialize the associated pointer list to contain the single number 0.

For $j := 1$ to m do

begin

Set k to be the first pointer on the b -pointer list.

$E(j) := \text{Cand}(k, j);$

$V(j) := \max[G(j), E(j), F(j)];$

{As before we assume that the needed F and G values have been computed.}

Convex gap weight

- Final implementation details

{Now see how j 's candidates change the block-partition.}

Set j' equal to the first entry on the end-of-block list.

{look for the first index s in the end-of-block list where j loses}

If $Cand(b(j'), j + 1) < Cand(j, j + 1)$ then { j 's candidate wins one}

begin

While

The end-of-block list is not empty and $Cand(b(j'), j') < Cand(j, j')$ do
begin

remove the first entry on the end-of-block list,
and remove the corresponding b -pointer

If the end-of-block list is not empty then
set j' to the new first entry on the end-of-block list.

end;

end {while};

Convex gap weight

- **Final implementation details**

If the end-of-block list is empty then
place m at the head of that list;

Else {when the end-of-block list is not empty}
begin

Let p_s denote the first end-of-block entry.

Using binary search over the cells in block s , find the
right-most point p in that block such that $Cand(j, p) > Cand(b_s, p)$.

Add p to the head of the end-of-block list;
end;

Add j to the head of the b pointer list.

end;

end.

Convex gap weight

- **Time analysis**
 - The total time for the algorithm
 - Proportional to the number of comparisons
 - Find block s $\sim l > 2$ comparisons, at least $l - 1$ full blocks coalesce into a single block
 - Binary search to split s \sim splits at most one block into two
 - Hence if the algorithm does $l > 2$ **comparisons** to find s ,
 - Then the total number of blocks **at most increases by one**.
 - The algorithm begins with a single block and n iterations
 - To find every s : At most $O(n)$ comparisons
 - To find split cell (binary search): $O(\log n)$
- **Theorem 12.6.1**
 - For any fixed row, all the $E(j)$ values can be computed in $O(n \log n)$ total time.

Convex gap weight

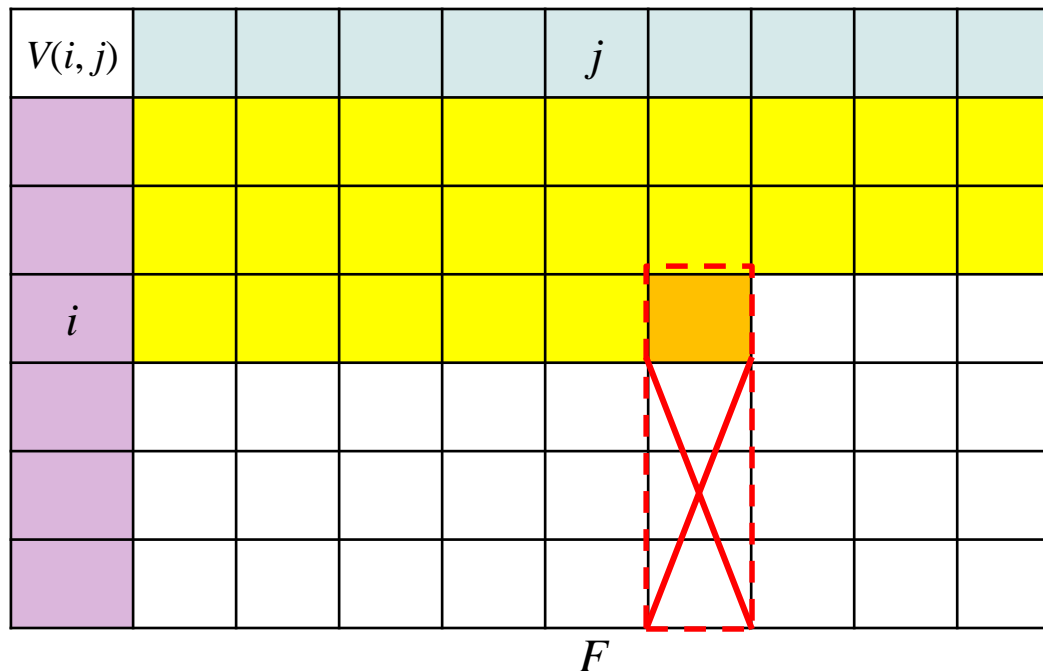
- The case of F values is essentially symmetric
 - One point that might cause confusion
 - The computations of E and F are actually *interleaved*
 - since each $V(i, j)$ value depends on both $E(i, j)$ and $F(i, j)$

$V(i, j)$					j				
i									

E

Convex gap weight

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Convex gap weight

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$V(i, j)$					j				
i									

F

Convex gap weight

- **Total time**
 - E value: $O(n \log n)$
 - F value: $O(m \log m)$
 - G value: $O(nm)$
 - V value: $O(nm)$ once E and F is known
- **Theorem 12.6.2**
 - When the gap weight w is a convex function of the gap length
 - An optimal alignment can be computed in $O(nm \log n)$ time
 - where $n > m$ are the lengths of the two strings