
Introduction to Algorithms

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Computational problems

- A computational problem specifies an input-output relationship
 - What does the input look like?
 - What should the output be for each input?
 - Example:
 - Input: an integer number N
 - Output: Is the number prime?
 - Example:
 - Input: A list of names of people
 - Output: The same list sorted alphabetically
 - Example:
 - Input: A picture in digital format
 - Output: An English description of what the picture shows
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Algorithms

- An algorithm is an exact specification of how to solve a computational problem
- An algorithm must specify every step completely, so a computer can implement it without any further “understanding”
- An algorithm must work for all possible inputs of the problem.
- Algorithms must be:
 - Correct: For each input, terminate and produce an appropriate output
 - Efficient: run as quickly as possible, and use as little memory as possible – more about this later
- There can be many different algorithms for each computational problem.

Describing Algorithms

- Algorithms can be implemented in any programming language
- Usually we use “pseudo-code” to describe algorithms

Testing whether input N is prime:

- ```
For j = 2 .. N-1
 If the remainder of j/N is 0
 Output "N is composite" and halt
Output "N is prime"
```

- In this course we will just describe algorithms in Perl and pseudocode
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# Greatest Common Divisor

- The first algorithm “invented” in history was Euclid’s algorithm for finding the greatest common divisor (GCD) of two natural numbers
  - **Definition:** The GCD of two natural numbers  $x, y$  is the largest integer  $j$  that divides both evenly (with remainder 0).
  - **The GCD Problem:**
    - Input: natural numbers  $x, y$
    - Output:  $GCD(x,y)$  – their GCD
-

# Euclid's GCD Algorithm

```
sub gcd {
 my ($x, $y) = @_; // retrieve input x and y
 while ($y != 0) { // while y is not equal to 0
 $t = $x % $y; // get the modulus of x and y
 $x = $y; // replace x by y
 $y = $t; // replace y by t
 }
 return $x; // return the result (gcd of x and y)
}

print gcd(14, 21), "\n";
```

# Euclid's GCD Algorithm – sample

```
while ($y != 0) { // while y is not equal to 0
 $t = $x % $y; // get the modulus of x and y
 $x = $y; // replace x by y
 $y = $t; // replace y by t
}
```

## Example: Computing GCD(48,120)

|                | t  | x   | y   |
|----------------|----|-----|-----|
| After 0 rounds | -- | 72  | 120 |
| After 1 round  | 72 | 120 | 72  |
| After 2 rounds | 48 | 72  | 48  |
| After 3 rounds | 24 | 48  | 24  |
| After 4 rounds | 0  | 24  | 0   |

Output: 24

# Termination of Euclid's Algorithm

- Why does this algorithm terminate?
  - After any iteration we have that  $x > y$  since the new value of  $y$  is the remainder of the division by the new value of  $x$ .
  - In further iterations, we replace  $(x, y)$  with  $(y, x\%y)$ , and  $x\%y < x$ , thus the numbers decrease in each iteration.
  - Formally, the value of  $xy$  decreases at each iteration (except, maybe, the first one). When it reaches 0, the algorithm must terminate.

```
sub gcd {
 my ($x, $y) = @_; // retrieve input x and y
 while ($y != 0) { // while y is not equal to 0
 $t = $x % $y; // get the modulus of x and y
 $x = $y; // replace x by y
 $y = $t; // replace y by t
 }
 return $x; // return the result (gcd of x and y)
}
```



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# Introduction to Algorithms

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Running Time Analysis

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# How fast will your program run?

- The running time of your program will depend upon:
    - ❑ The algorithm
    - ❑ The input
    - ❑ Your implementation of the algorithm in a programming language
    - ❑ The compiler you use
    - ❑ The operating system (OS) on your computer
    - ❑ Your computer hardware
    - ❑ Maybe other things: temperature outside; other programs on your computer; ...
  - Our Motivation: analyze the running time of an algorithm as a function of only simple parameters of the input.
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# Basic idea: counting operations

- Each algorithm performs a sequence of basic operations:
    - Arithmetic:  $(\text{low} + \text{high})/2$
    - Comparison: `if ( x > 0 ) ...`
    - Assignment: `temp = x`
    - Branching: `while ( y != 0 ) { ... }`
    - ...
  - Idea: count the number of basic operations performed on the input.
  - Difficulties:
    - Which operations are basic?
    - Not all operations take the same amount of time.
    - Operations take different times with different hardware or compilers
-

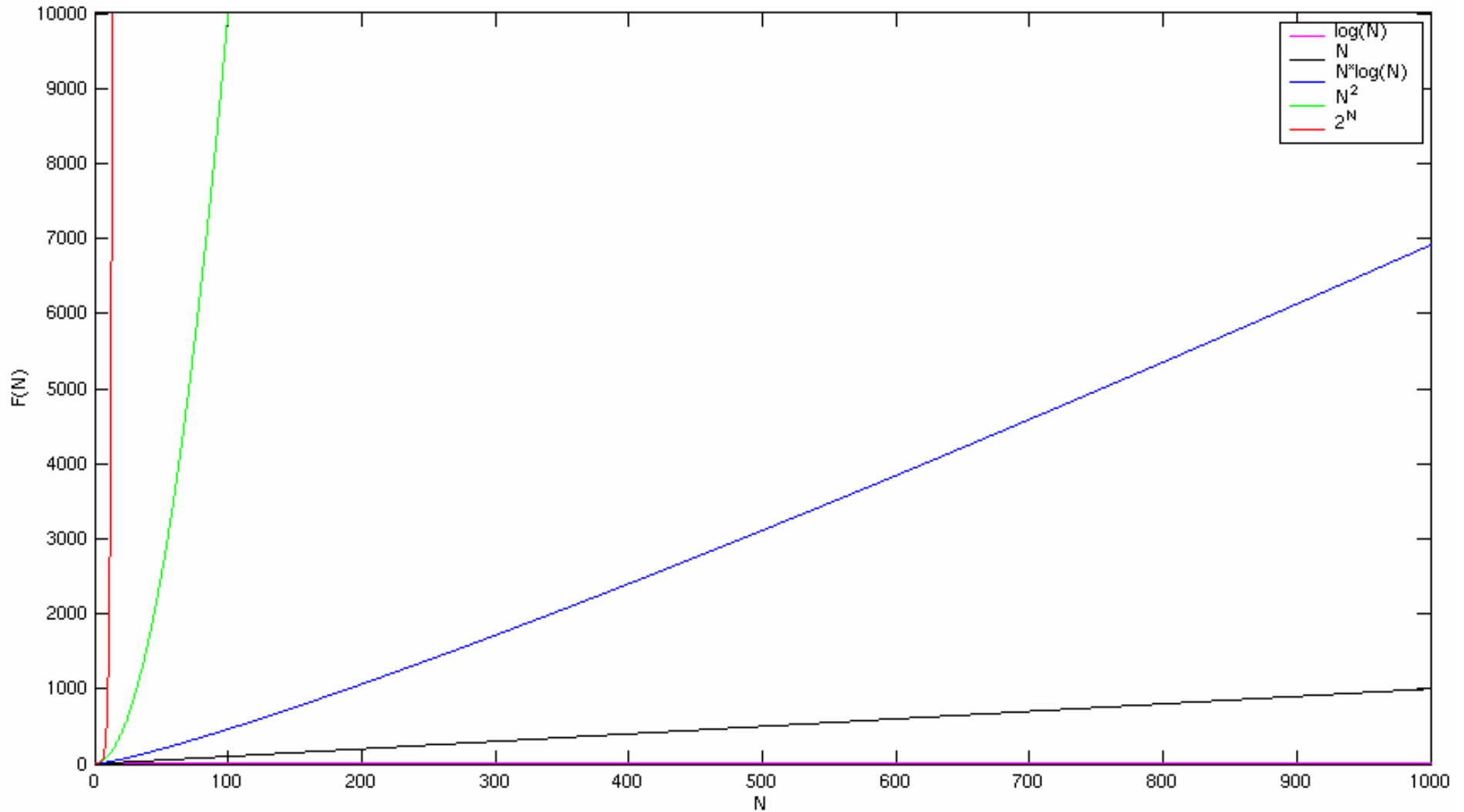
# Asymptotic running times

- Operation counts are only problematic in terms of constant factors.
- The general form of the function describing the running time is invariant over hardware, languages or compilers!

```
sub myMethod{
 my $N = shift @_;
 my $sq = 0;
 for($j=0; $j <$N ; $j++)
 for($k=0; $k<$N ; $k++)
 $sq++;
 return $sq;
}
```

- Running time is “about”  $N^2$ .
- We use “Big-O” notation, and say that the running time is  $O(N^2)$

# Asymptotic behavior of functions



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# Mathematical Formalization

- Definition: Let  $f$  and  $g$  be functions from the natural numbers to the natural numbers. We write  $f=O(g)$  if there exists a constant  $c$  such that for all  $n$ :  $f(n) \leq cg(n)$ .

$$f=O(g) \Leftrightarrow \exists c \forall n: f(n) \leq cg(n)$$

- This is a mathematically formal way of ignoring constant factors, and looking only at the “shape” of the function.
  - $f=O(g)$  should be considered as saying that “ $f$  is at most  $g$ , up to constant factors”.
  - We usually will have  $f$  be the running time of an algorithm and  $g$  a nicely written function. E.g. The running time of the previous algorithm was  $O(N^2)$ .
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# Asymptotic analysis of algorithms

- We usually embark on an *asymptotic worst case* analysis of the running time of the algorithm.
  - Asymptotic:
    - Formal, exact, depends only on the algorithm
    - Ignores constants
    - Applicable mostly for large input sizes
  - Worst Case:
    - Bounds on running time must hold for *all* inputs.
    - Thus the analysis considers the worst-case input.
    - Sometimes the “average” performance can be much better
    - Real-life inputs are rarely “average” in any formal sense
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# The running time of Euclid's GCD Algorithm

- How fast does Euclid's algorithm terminate?
  - After the first iteration we have that  $x > y$ . In each iteration, we replace  $(x, y)$  with  $(y, x \% y)$ .
  - In an iteration where  $x > 1.5y$  then  $x \% y < y < 2x/3$ .
  - In an iteration where  $x \leq 1.5y$  then  $x \% y \leq y/2 < 2x/3$ .
  - Thus, the value of  $xy$  decreases by a factor of at least  $2/3$  each iteration (except, maybe, the first one).

```
sub gcd {
 my ($x, $y) = @_; // retrieve input x and y
 while ($y != 0) { // while y is not equal to 0
 $t = $x % $y; // get the modulus of x and y
 $x = $y; // replace x by y
 $y = $t; // replace y by t
 }
 return $x; // return the result (gcd of x and y)
}
```



# The running time of Euclid's Algorithm

- Theorem: Euclid's GCD algorithm runs in time  $O(N)$ , where  $N$  is the input length ( $N = \log_2 x + \log_2 y$ ).
- Proof:
  - Every iteration of the loop (except maybe the first) the value of  $xy$  decreases by a factor of at least  $2/3$ . Thus after  $k+1$  iterations the value of  $xy$  is at most  $(2/3)^k$  the original value.
  - Thus the algorithm must terminate when  $k$  satisfies:  $xy(2/3)^k < 1$  (for the original values of  $x, y$ ).
  - Thus the algorithm runs for at most  $1 + \log_{3/2} xy$  iterations.
  - Each iteration has only a constant  $L$  number of operations, thus the total number of operations is at most  $(1 + \log_{3/2} xy)L$
  - Formally,  $(1 + \log_{3/2} xy)L \leq L(1 + 2\log_2 x + 2\log_2 y) \leq 3LN$
  - Thus the running time is  $O(N)$ .

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# Introduction to Algorithms

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Recursion

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# Designing Algorithms

- There is no single recipe for inventing algorithms
- There are basic rules:
  - Understand your problem well – may require much mathematical analysis!
  - Use existing algorithms (reduction) or algorithmic ideas
- There is a single basic algorithmic technique:

## Divide and Conquer

- In its simplest (and most useful) form it is simple induction
    - In order to solve a problem, solve a similar problem of smaller size
  - The key conceptual idea:
    - Think only about how to use the smaller solution to get the larger one
    - Do not worry about how to solve the smaller problem (it will be solved using an even smaller one)
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# Recursion

- A recursive method is a method that contains a call to itself
  - Technically:
    - All modern computing languages allow writing methods that call themselves
    - We will discuss how this is implemented later
  - Conceptually:
    - This allows programming in a style that reflects divide-n-conquer algorithmic thinking
    - At the beginning recursive programs are confusing – after a while they become clearer than non-recursive variants
-

# Factorial

```
sub factorial {
 my $n = shift @_; // retrieve input
 if ($n == 0) {
 return 1; // if input is 0, return 1
 } else {
 // otherwise, compute the factorial of $n-1,
 // multiply it by $n and return the product
 return $n * factorial($n-1);
 }
}

print "5! = ", factorial(5), "\n";
```

---

# Elements of a recursive program

- **Basis:** a case that can be answered without using further recursive calls
    - In our case: `if ($n==0) { return 1; }`
  - **Creating the smaller problem, and invoking a recursive call on it**
    - In our case: `factorial($n-1)`
  - **Finishing to solve the original problem**
    - In our case: `return $n; //solution of recursive call`
-

# Tracing the factorial method

```
print "5! = ", factorial(5), "\n";

 5 * factorial(4)
 4 * factorial(3)
 3 * factorial(2)
 2 * factorial(1)
 1 * factorial(0)
 return 1
 return 1
 return 2
 return 6
 return 24
 return 120
```

# Correctness of factorial method

- Theorem: For every positive integer  $n$ , factorial ( $n$ ) returns the value  $n!$ .
- Proof: By induction on  $n$ :
- Basis: for  $n=0$ , factorial ( $0$ ) returns  $1=0!$ .
- Induction step: When called on  $n>1$ , factorial calls factorial ( $n-1$ ), which by the induction hypothesis returns  $(n-1)!$ . The returned value is thus  $n*(n-1)!=n!$ .



# Raising to power – take 1

```
sub power {
 my ($x, $n) = @_; // retrieve the input
 if ($n == 0) { // if $n is 0, return 1
 return 1.0;
 }
 // otherwise, return $x multiplied by the
 // result of power of x to the (n-1)th
 return $x * power($x, $n-1);
}

print "3^9 = ", power(3, 9), "\n";
```

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# Running time analysis

- Simplest way to calculate the running time of a recursive program is to add up the running times of the separate levels of recursion.
  - In the case of the power method:
    - There are  $n+1$  levels of recursion
      - $\text{power}(x,n), \text{power}(x,n-1), \text{power}(x, n-2), \dots \text{power}(x,0)$
    - Each level takes  $O(1)$  steps
    - Total time =  $O(n)$
-

# Raising to power – take 2

```
sub power2 {
 my ($x, $n) = @_;
 if ($n == 0) {
 return 1.0;
 }
 if ($n%2 == 0) {
 my $t = power2($x, $n/2);
 return $t*$t;
 }
 return $x * power2($x, $n-1);
}
```

# Analysis

- Theorem: For any  $x$  and positive integer  $n$ , the power method returns  $x^n$ .
- Proof: by complete induction on  $n$ .
  - Basis: For  $n=0$ , we return 1.
  - If  $n$  is even, we return  $\text{power}(x, n/2) * \text{power}(x, n/2)$ . By the induction hypothesis  $\text{power}(x, n/2)$  returns  $x^{n/2}$ , so we return  $(x^{n/2})^2 = x^n$ .
  - If  $n$  is odd, we return  $x * \text{power}(x, n-1)$ . By the induction hypothesis  $\text{power}(x, n-1)$  returns  $x^{n-1}$ , so we return  $x \cdot x^{n-1} = x^n$ .
- The running time is now  $O(\log n)$ :
  - After 2 levels of recursion  $n$  has decreased by a factor of at least two (since either  $n$  or  $n-1$  is even, in which case the recursive call is with  $n/2$ )
  - Thus we reach  $n==0$  after at most  $2\log_2 n$  levels of recursion
  - Each level still takes  $O(1)$  time.

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# Introduction to Algorithms

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Algorithms for bioinformatics

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# Bring in the Bioinformaticians

- Gene similarities between two genes with known and unknown function alert biologists to some possibilities
  - Computing a similarity score between two genes tells how likely it is that they have similar functions
  - **Dynamic programming** is a technique for revealing similarities between genes
  - The ***Change Problem*** is a good problem to introduce the idea of dynamic programming
-

# The Change Problem

**Goal**: Convert some amount of money  $M$  into given denominations, using the fewest possible number of coins

**Input**: An amount of money  $M$ , and an array of  $d$  denominations  $\mathbf{c} = (c_1, c_2, \dots, c_d)$ , in a decreasing order of value ( $c_1 > c_2 > \dots > c_d$ )

**Output**: A list of  $d$  integers  $i_1, i_2, \dots, i_d$  such that

$$c_1 i_1 + c_2 i_2 + \dots + c_d i_d = M$$

and  $i_1 + i_2 + \dots + i_d$  is minimal

# Change Problem: Example

Given the denominations 1, 3, and 5, what is the minimum number of coins needed to make change for a given value?

| Value          | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|---|---|---|---|---|---|---|---|---|----|
| Min # of coins | 1 |   | 1 |   | 1 |   |   |   |   |    |

Only one coin is needed to make change for the values 1, 3, and 5



# Change Problem: Example (cont'd)

Given the denominations 1, 3, and 5, what is the minimum number of coins needed to make change for a given value?

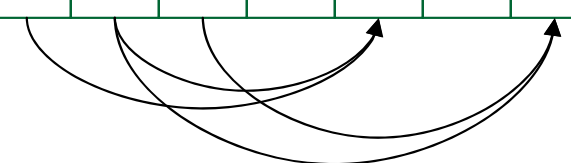
| Value          | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|---|---|---|---|---|---|---|---|---|----|
| Min # of coins | 1 | 2 | 1 | 2 | 1 | 2 |   | 2 |   | 2  |

However, two coins are needed to make change for the values 2, 4, 6, 8, and 10.

# Change Problem: Example (cont'd)

Given the denominations 1, 3, and 5, what is the minimum number of coins needed to make change for a given value?

| Value          | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|----------------|---|---|---|---|---|---|---|---|---|----|
| Min # of coins | 1 | 2 | 1 | 2 | 1 | 2 | 3 | 2 | 3 | 2  |



Lastly, three coins are needed to make change for the values 7 and 9

# Change Problem: Recurrence

This example is expressed by the following recurrence relation:

$$\mathit{minNumCoins}(M) = \mathbf{\min\ of} \left\{ \begin{array}{l} \mathit{minNumCoins}(M-1) + 1 \\ \mathit{minNumCoins}(M-3) + 1 \\ \mathit{minNumCoins}(M-5) + 1 \end{array} \right.$$

Given the denominations  $\mathbf{c}$ :  $c_1, c_2, \dots, c_d$ , the recurrence relation is:

$$\mathit{minNumCoins}(M) = \mathbf{\min\ of} \left\{ \begin{array}{l} \mathit{minNumCoins}(M-c_1) + 1 \\ \mathit{minNumCoins}(M-c_2) + 1 \\ \dots \\ \mathit{minNumCoins}(M-c_d) + 1 \end{array} \right.$$

# Change Problem: A Recursive Algorithm

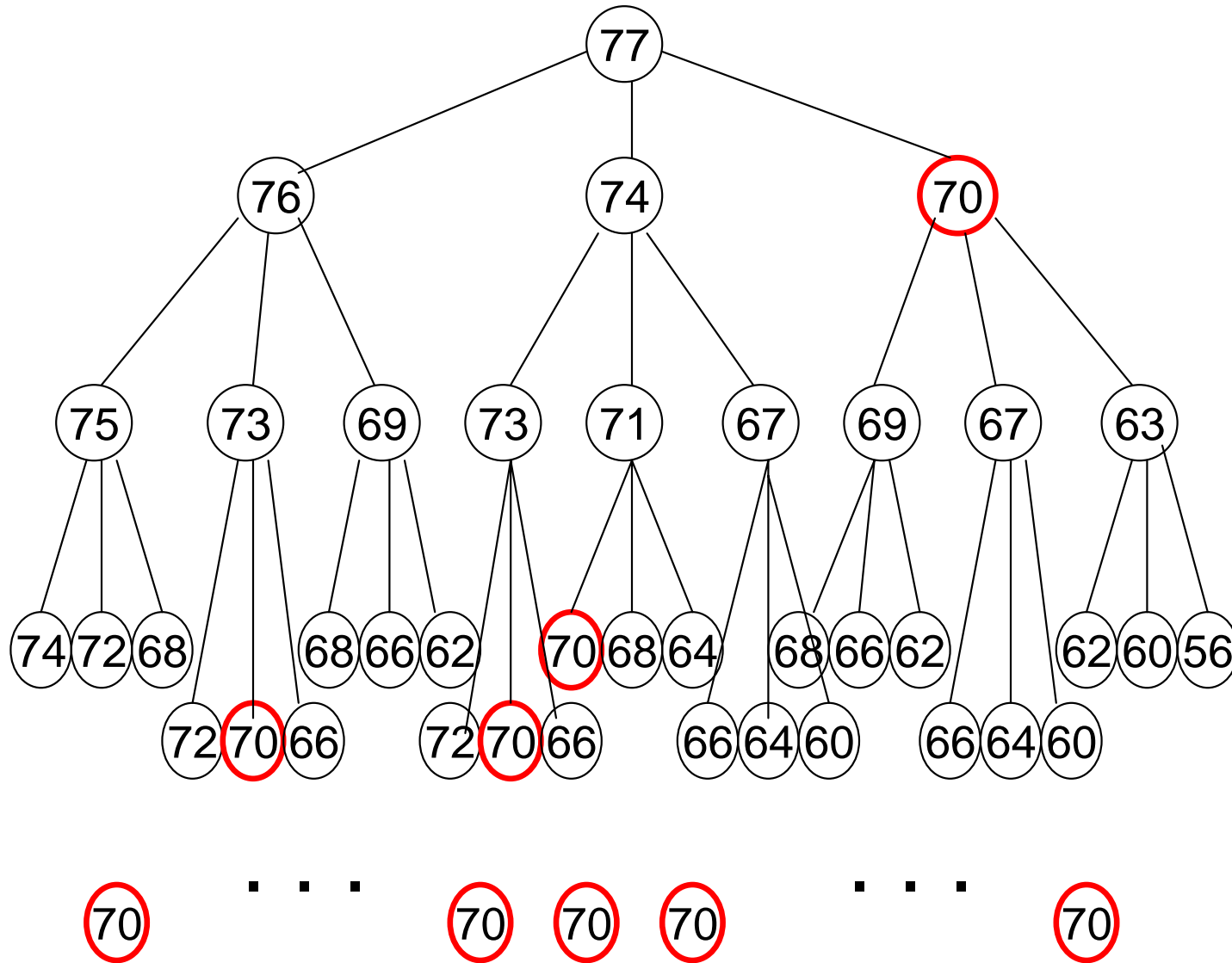
1. RecursiveChange( $M, c, d$ )
2.     if  $M = 0$
3.         return 0
4.      $bestNumCoins = \text{infinity}$
5.     for  $i = 1$  to  $d$
6.         if  $M \geq c_i$
7.              $numCoins = \text{RecursiveChange}(M - c_i, c, d)$
8.             if  $numCoins + 1 < bestNumCoins$
9.                  $bestNumCoins = numCoins + 1$
10.     return  $bestNumCoins$

---

# RecursiveChange Is Not Efficient

- It recalculates the optimal coin combination for a given amount of money repeatedly
  - i.e.,  $M = 77$ ,  $c = (1,3,7)$ :
    - Optimal coin combo for 70 cents is computed **9** times!
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# The RecursiveChange Tree



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# We Can Do Better

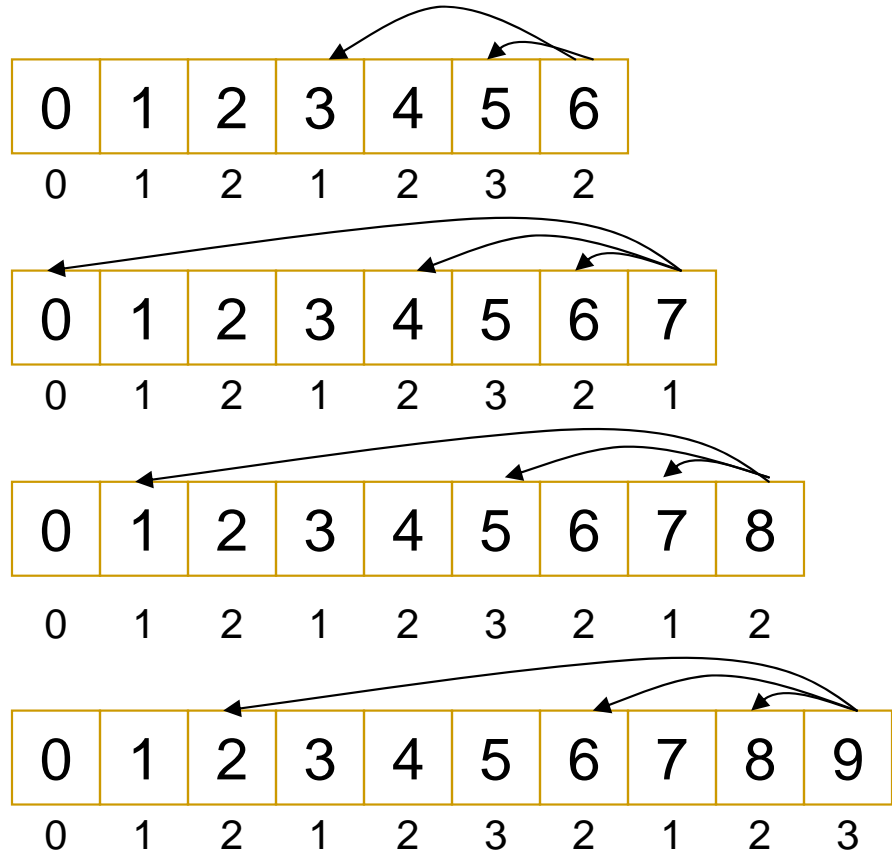
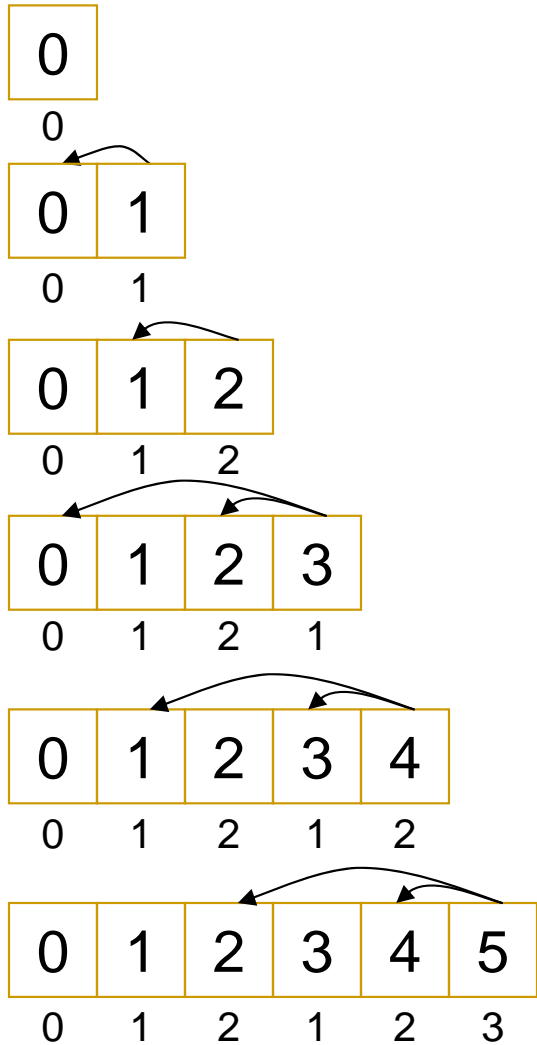
- We're re-computing values in our algorithm more than once
  - Save results of each computation for 0 to  $M$
  - This way, we can do a reference call to find an already computed value, instead of re-computing each time
  - Running time becomes  $M^* d$ , where  $M$  is the value of money and  $d$  is the number of denominations
-

# The Change Problem: Dynamic Programming

1. DPChange( $M, c, d$ )
2.  $bestNumCoins_0 = 0$
3. for  $m = 1$  to  $M$
4.  $bestNumCoins_m = \text{infinity}$
5. for  $i = 1$  to  $d$
6. if  $m \geq c_i$
7. if  $bestNumCoins_{m - c_i} + 1 < bestNumCoins_m$
8.  $bestNumCoins_m = bestNumCoins_{m - c_i} + 1$
9. return  $bestNumCoins_M$



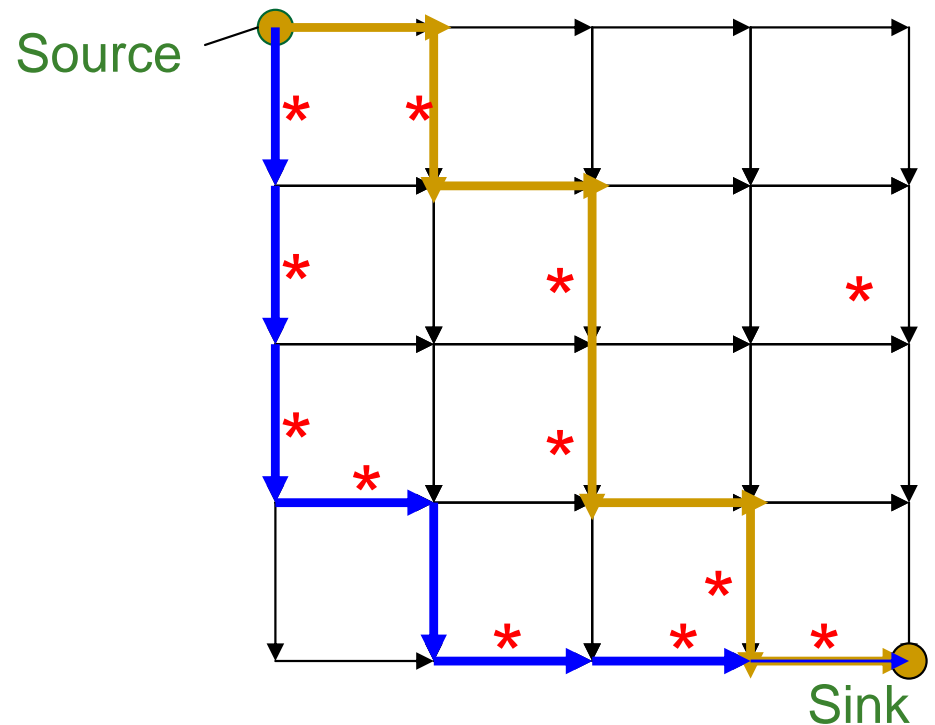
# DPChange: Example



$$\mathbf{c} = (1, 3, 7)$$
$$\mathbf{M} = 9$$

# Manhattan Tourist Problem (MTP)

Imagine seeking a path (from source to sink) to travel (only eastward and southward) with the most number of attractions (\*) in the Manhattan grid



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## Manhattan Tourist Problem: Formulation

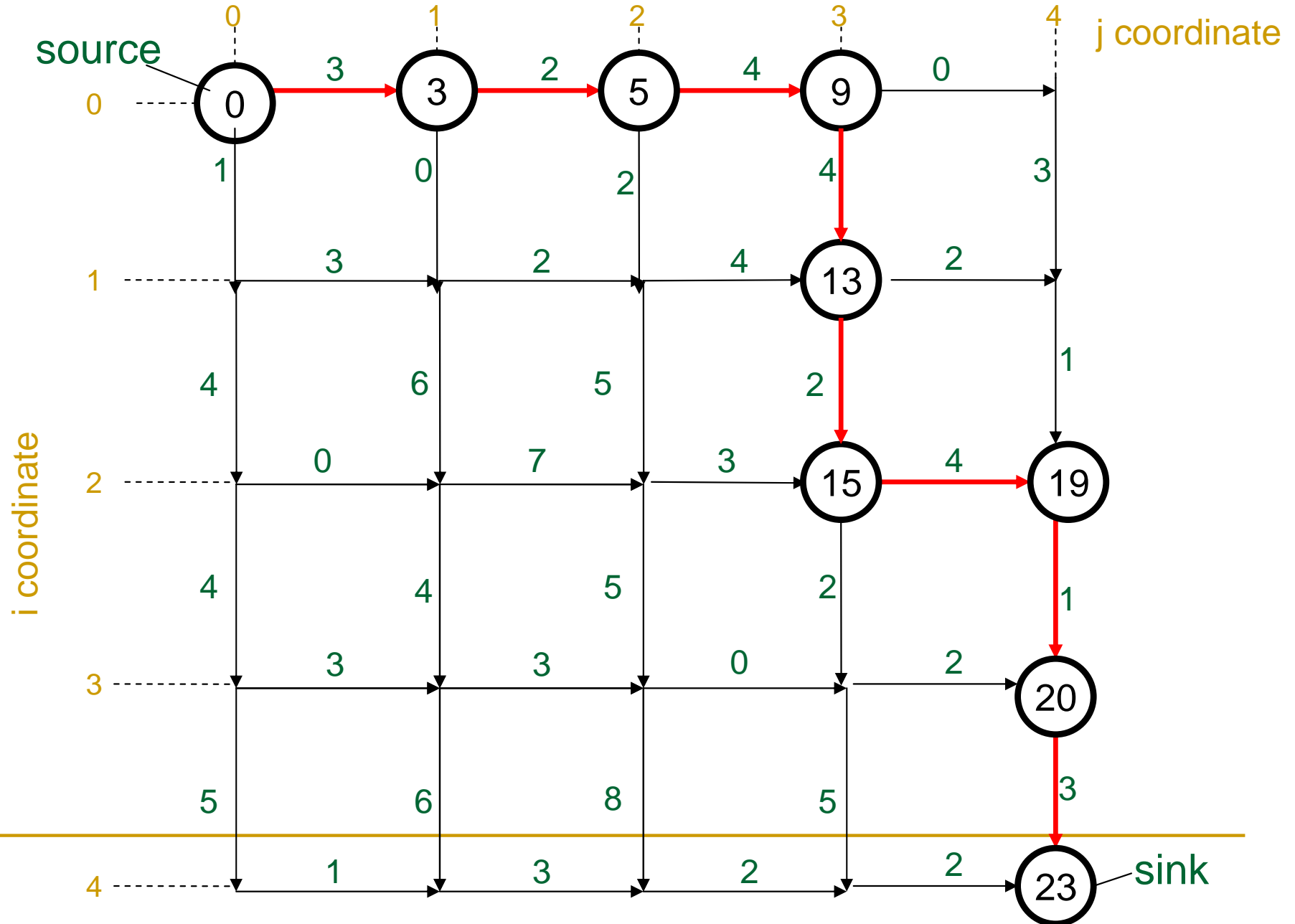
Goal: Find the longest path in a weighted grid.

Input: A weighted grid  $\mathbf{G}$  with two distinct vertices, one labeled “*source*” and the other labeled “*sink*”

Output: A longest path in  $\mathbf{G}$  from “*source*” to “*sink*”

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# MTP: An Example



# MTP: Simple Recursive Program

MT( $n, m$ )

if  $n=0$  or  $m=0$

return  $MT(n, m)$

$x = MT(n-1, m) +$

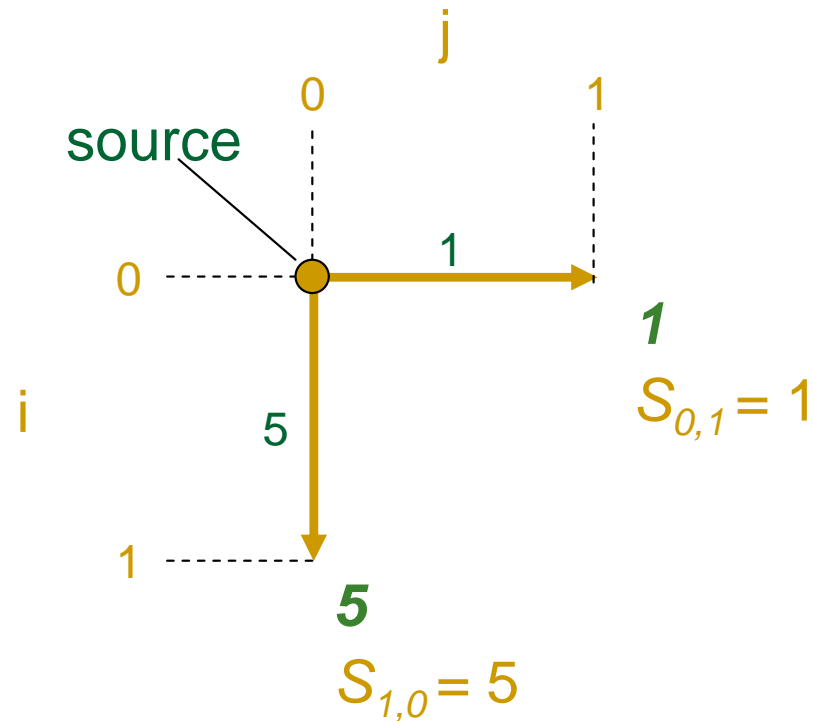
length of the edge from  $(n-1, m)$  to  $(n, m)$

$y = MT(n, m-1) +$

length of the edge from  $(n, m-1)$  to  $(n, m)$

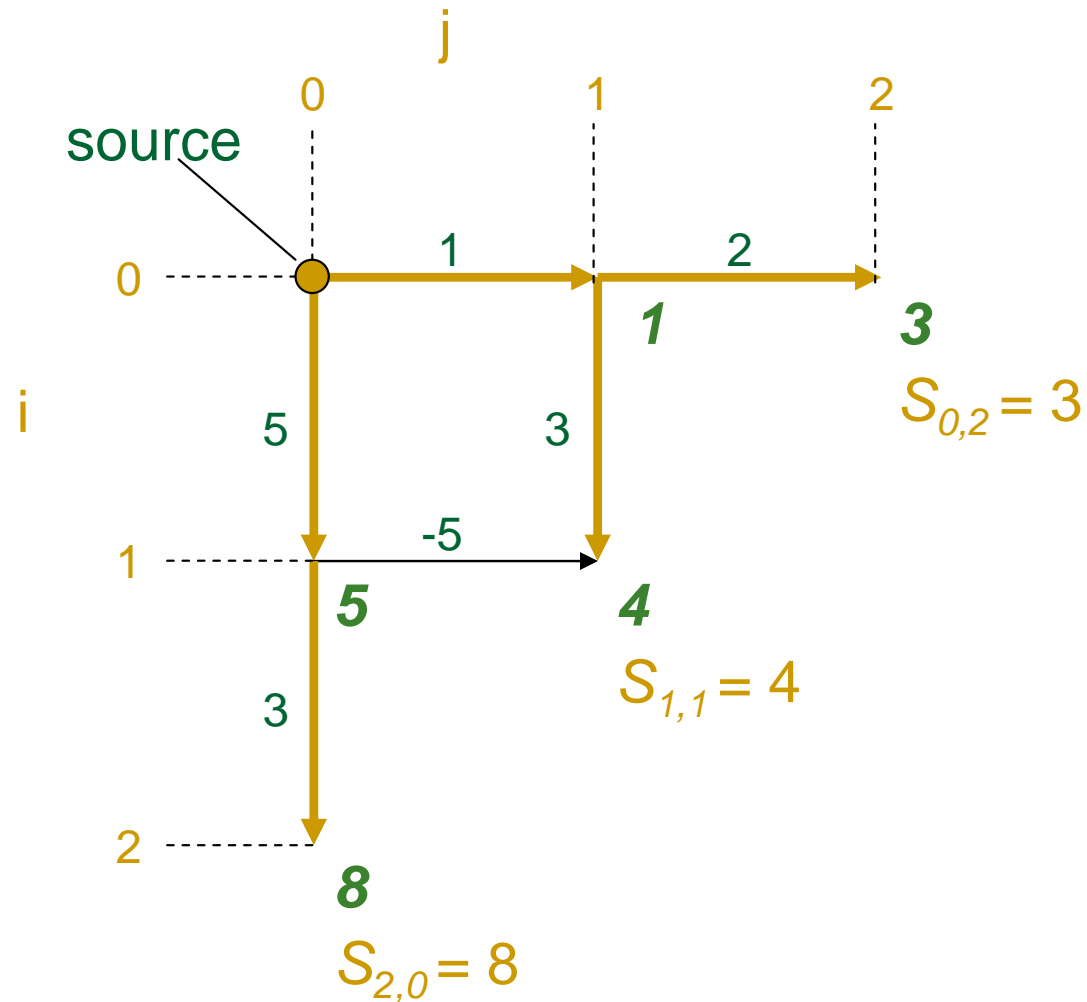
return  $\max\{x, y\}$

# MTP: Dynamic Programming

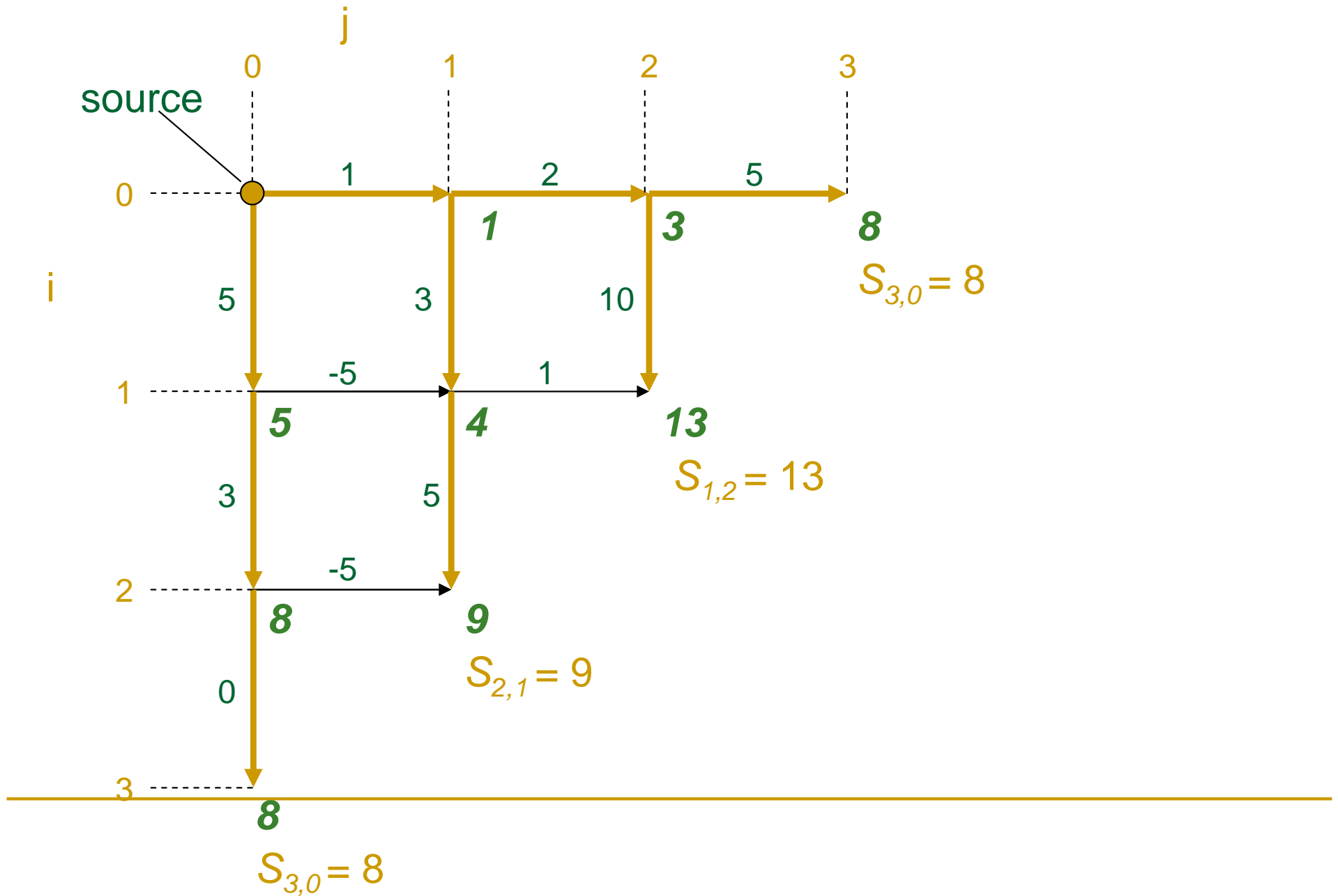


- Calculate optimal path score for each vertex in the graph
- Each vertex's score is the maximum of the prior vertices score plus the weight of the respective edge in between

# MTP: Dynamic Programming (cont'd)

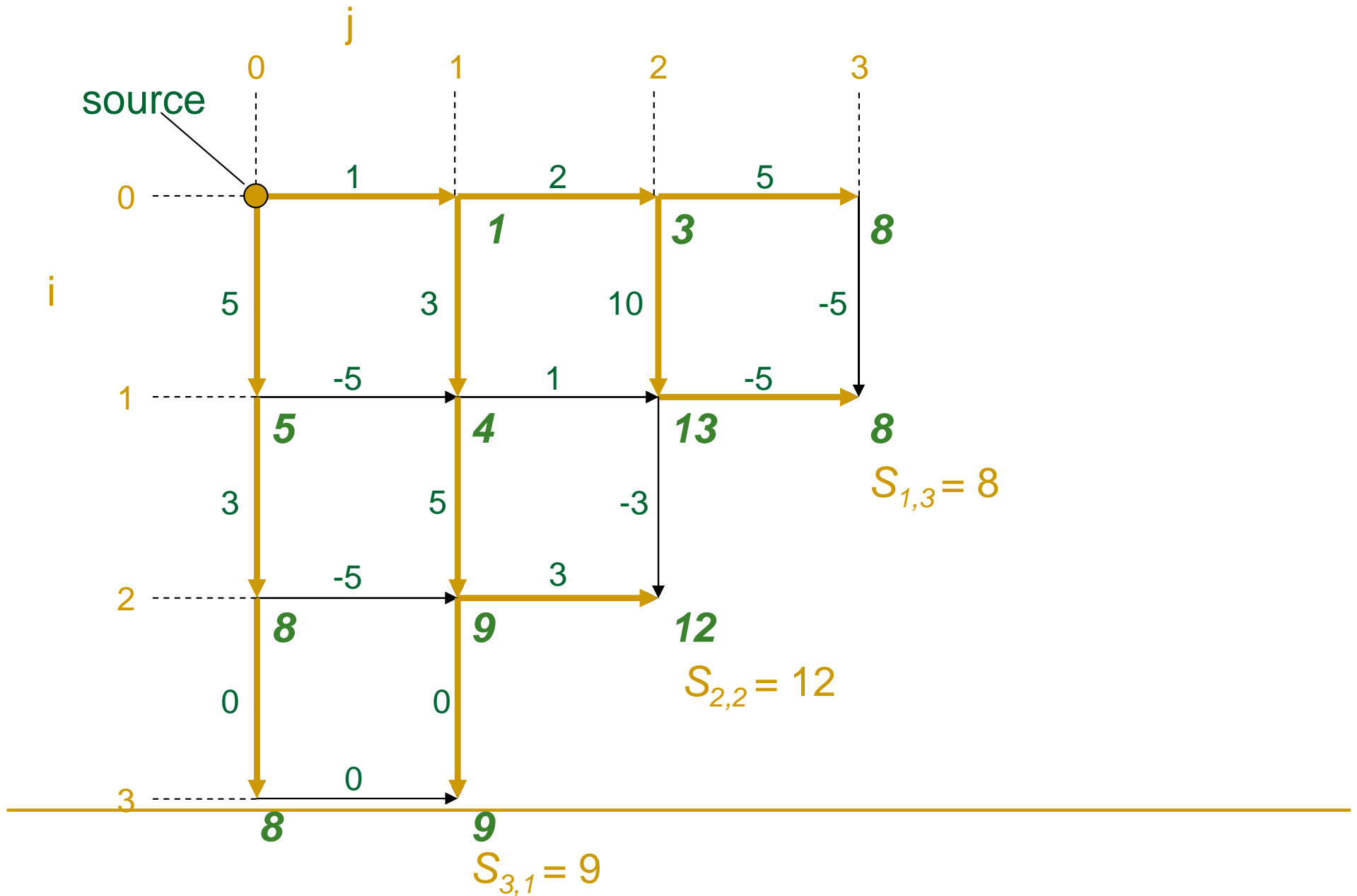


# MTP: Dynamic Programming (cont'd)

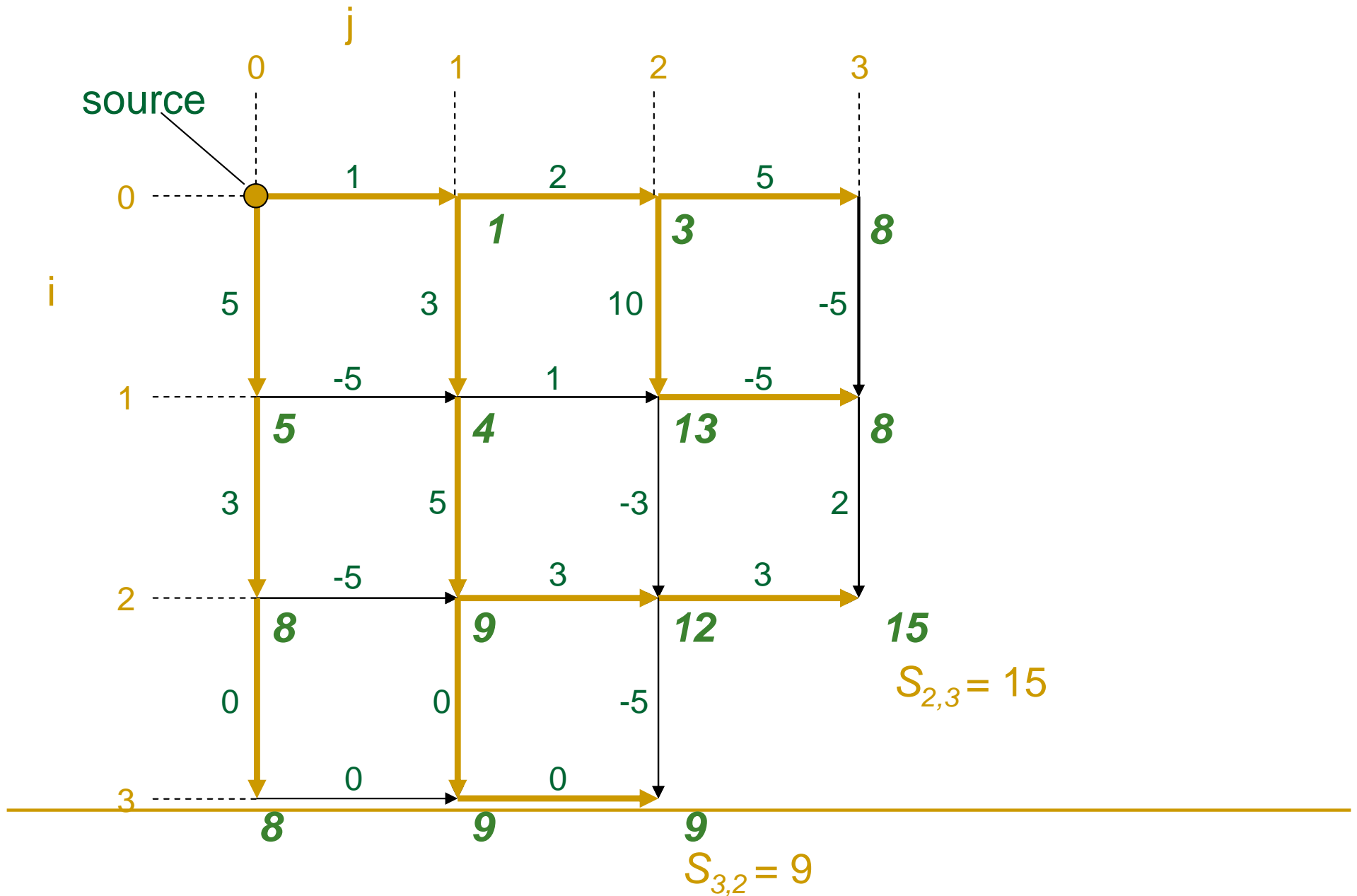




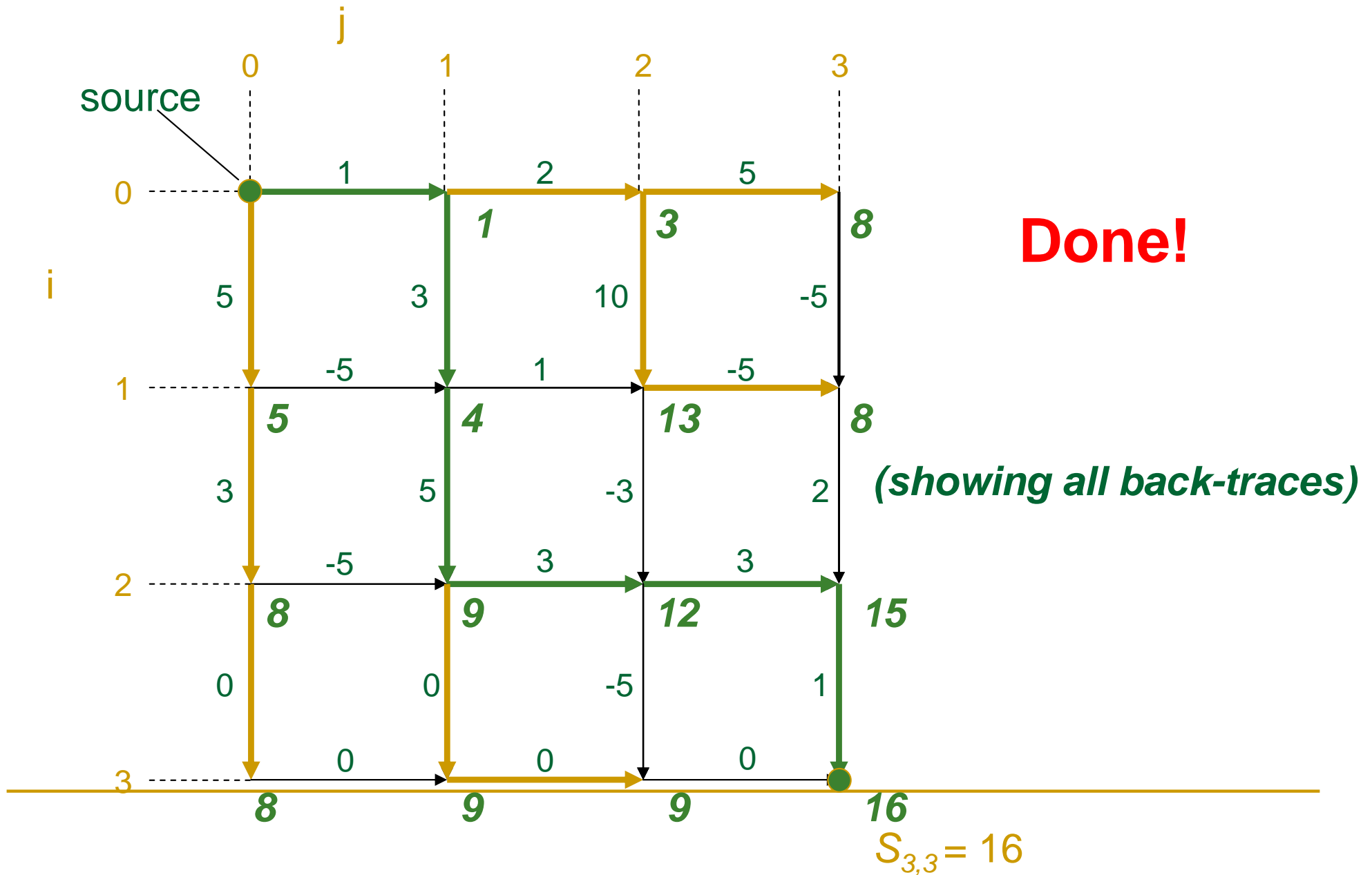
# MTP: Dynamic Programming (cont'd)



# MTP: Dynamic Programming (cont'd)



# MTP: Dynamic Programming (cont'd)



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# MTP: Recurrence

Computing the score for a point  $(i,j)$  by the recurrence relation:

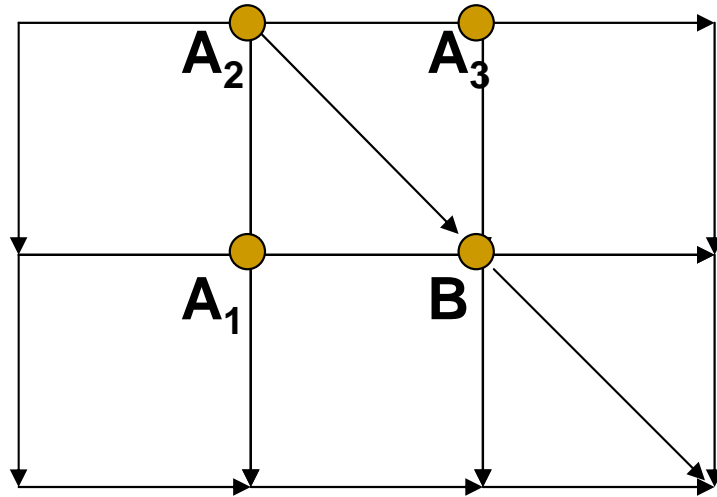
$$s_{i,j} = \max \left\{ \begin{array}{l} s_{i-1,j} + \text{weight of the edge between } (i-1, j) \text{ and } (i, j) \\ s_{i,j-1} + \text{weight of the edge between } (i, j-1) \text{ and } (i, j) \end{array} \right.$$

The running time is  $n \times m$  for a  $n$  by  $m$  grid

( $n = \#$  of rows,  $m = \#$  of columns)

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# Manhattan Is Not A Perfect Grid



What about diagonals?

- The score at point B is then given by:

$$s_B = \max \text{ of } \begin{cases} s_{A_1} + \text{weight of the edge } (A_1, B) \\ s_{A_2} + \text{weight of the edge } (A_2, B) \\ s_{A_3} + \text{weight of the edge } (A_3, B) \end{cases}$$

## Manhattan Is Not A Perfect Grid (cont'd)

Computing the score for point  $x$  is given by the recurrence relation:

$$s_x = \max_{\text{of}} \left\{ s_y + \text{weight of vertex } (y, x) \text{ where } y \in \text{Predecessors}(x) \right.$$

- Predecessors ( $x$ ) = set of vertices that have edges leading to  $x$
- The running time for a graph  $G(\mathbf{V}, \mathbf{E})$  ( $\mathbf{V}$  is the set of all vertices and  $\mathbf{E}$  is the set of all edges) is  $O(\mathbf{E})$  since each edge is evaluated once

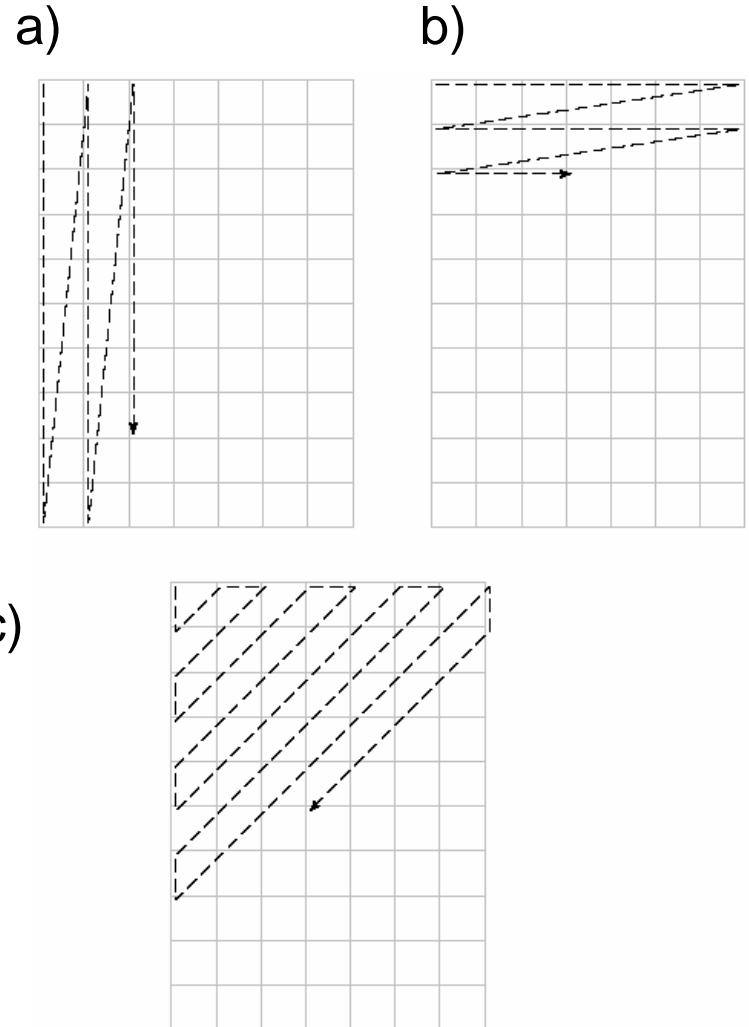
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## Traveling in the Grid

- The only hitch is that one must decide on the order in which to visit the vertices
  - By the time the vertex  $x$  is analyzed, the values  $s_y$  for all its predecessors  $y$  should be computed – otherwise we are in trouble.
  - We need to traverse the vertices in some order
-

# Traversing the Manhattan Grid

- 3 different strategies:
  - a) Column by column
  - b) Row by row
  - c) Along diagonals





# Alignment: 2 row representation

Given 2 DNA sequences  $v$  and  $w$ :

$v$  : **A** **T** **C** **T** **G** **A** **T**      $m = 7$   
 $w$  : **T** **G** **C** **A** **T** **A**      $n = 6$

Alignment :  $2 * k$  matrix (  $k \geq \max(m, n)$  )

|                |   |   |    |   |   |    |   |    |    |
|----------------|---|---|----|---|---|----|---|----|----|
| letters of $v$ | A | T | -- | G | T | T  | A | T  | -- |
| letters of $w$ | A | T | C  | G | T | -- | A | -- | C  |

4 matches

2 insertions

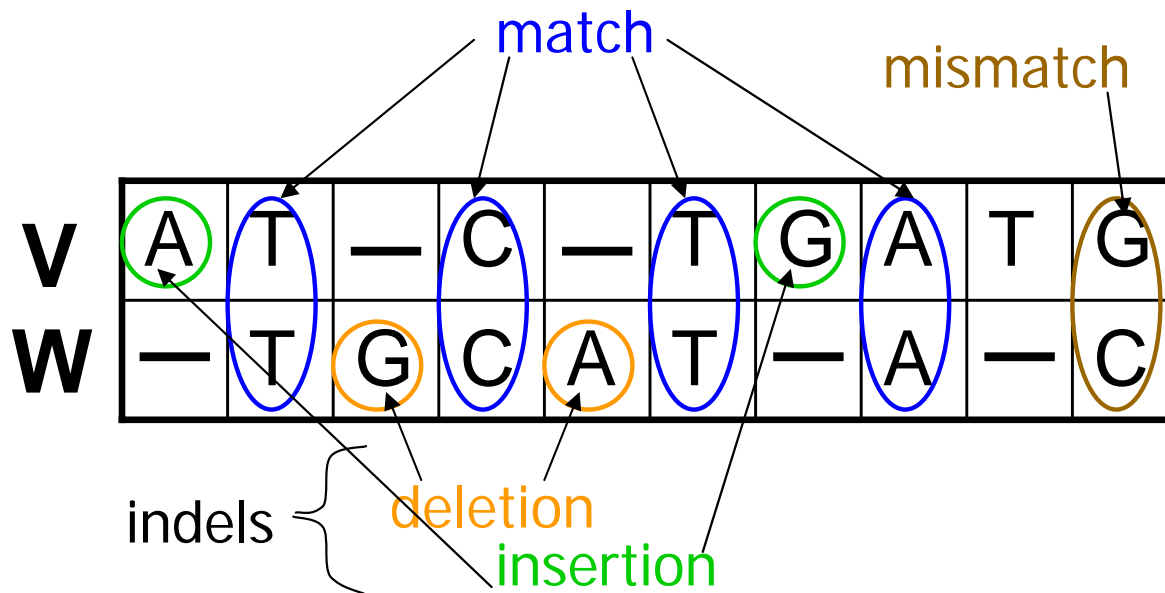
2 deletions

# Aligning DNA Sequences

**V** = ATCTGATG       $n = 8$

**W** = TGCATAC       $m = 7$

4 matches  
1 mismatches  
2 insertions  
2 deletions



Note:  
insertions and  
deletions are  
together  
called **indels**

# Longest Common Subsequence (LCS) – Alignment without Mismatches

- Given two sequences

$$\mathbf{v} = v_1 v_2 \dots v_m \text{ and } \mathbf{w} = w_1 w_2 \dots w_n$$

- The LCS of  $\mathbf{v}$  and  $\mathbf{w}$  is a sequence of positions in

$$\mathbf{v}: 1 \leq i_1 < i_2 < \dots < i_t \leq m$$

and a sequence of positions in

$$\mathbf{w}: 1 \leq j_1 < j_2 < \dots < j_t \leq n$$

such that  $i_t$ -th letter of  $\mathbf{v}$  equals to  $j_t$ -letter of  $\mathbf{w}$  and  $t$  is maximal

# LCS: Example

|                      |    |   |    |   |    |   |    |   |    |   |   |
|----------------------|----|---|----|---|----|---|----|---|----|---|---|
| <i>i</i> coords:     | 0  | 1 | 2  | 2 | 3  | 3 | 4  | 5 | 6  | 7 | 8 |
| elements of <i>v</i> | A  | T | -- | C | -- | T | G  | A | T  | C |   |
| elements of <i>w</i> | -- | T | G  | C | A  | T | -- | A | -- | C |   |
| <i>j</i> coords:     | 0  | 0 | 1  | 2 | 3  | 4 | 5  | 5 | 6  | 6 | 7 |

$(0,0) \rightarrow (1,0) \rightarrow (2,1) \rightarrow (2,2) \rightarrow (3,3) \rightarrow (3,4) \rightarrow (4,5) \rightarrow (5,5) \rightarrow (6,6) \rightarrow (7,6) \rightarrow (8,7)$

Matches shown in red

positions in *v*:  $2 < 3 < 4 < 6 < 8$

positions in *w*:  $1 < 3 < 5 < 6 < 7$

Every common subsequence is a path in 2-D grid

# LCS: Dynamic Programming

- Find the LCS of two strings

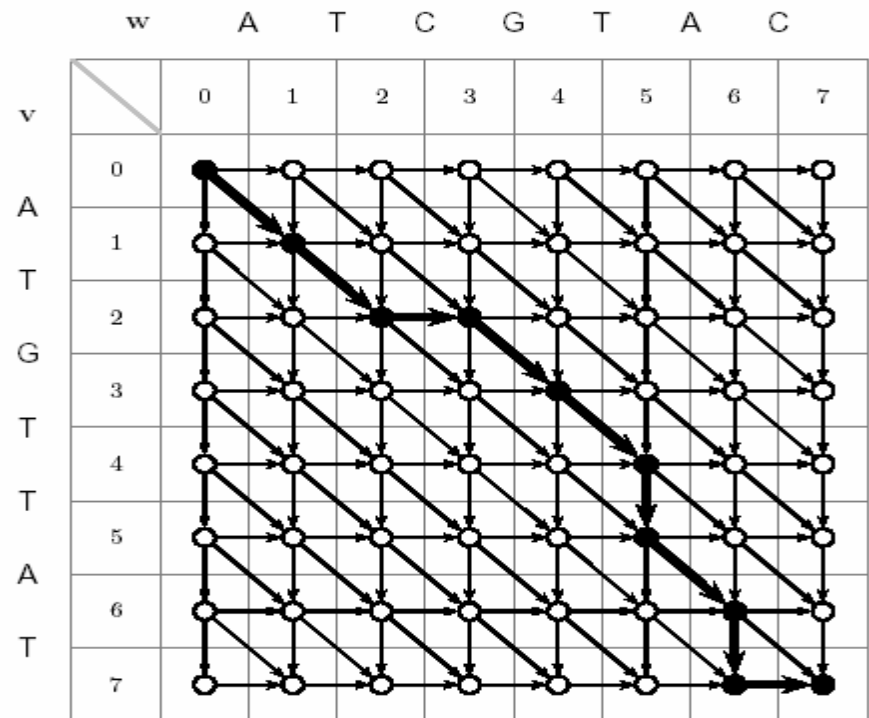
Input: A weighted graph  $G$  with two distinct vertices, one labeled “*source*” one labeled “*sink*”

Output: A longest path in  $G$  from “*source*” to “*sink*”

```

v = 0 1 2 2 3 4 5 6 7 7
 | | | | | | | | |
w = A T C G T - A - C
 0 1 2 3 4 5 5 6 6 7

```

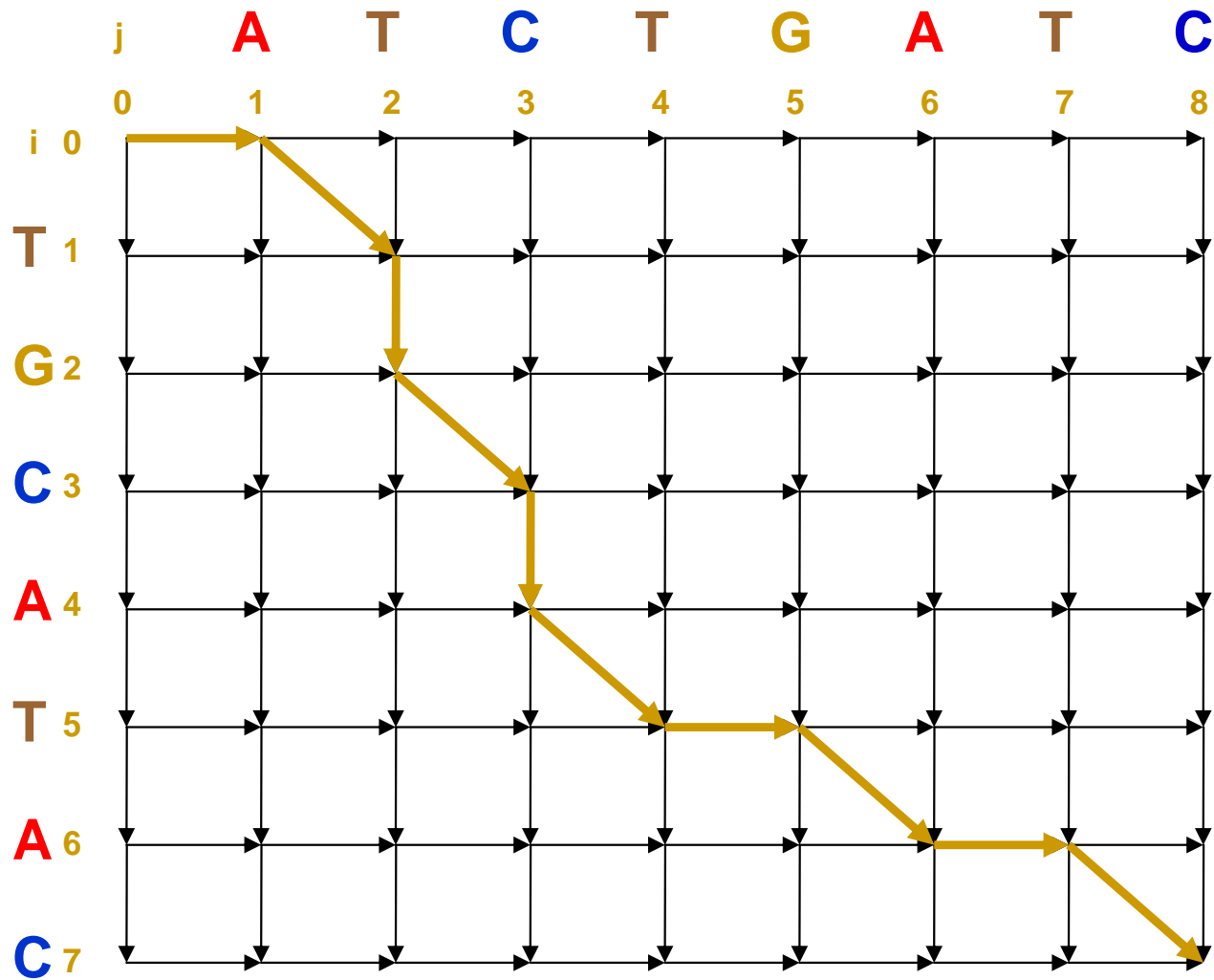


```

 ↘ ↘ → ↘ ↘ ↓ ↘ ↓ →
 A T - G T T A T -
 A T C G T - A - C

```

# LCS Problem as Manhattan Tourist Problem



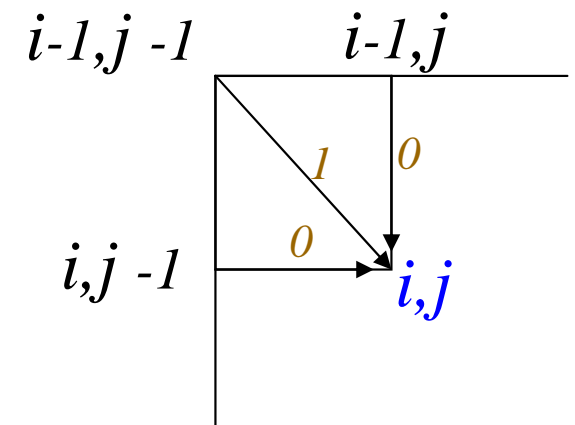
# Computing LCS

Let  $\mathbf{v}_i =$  prefix of  $\mathbf{v}$  of length  $i$ :  $v_1 \dots v_i$

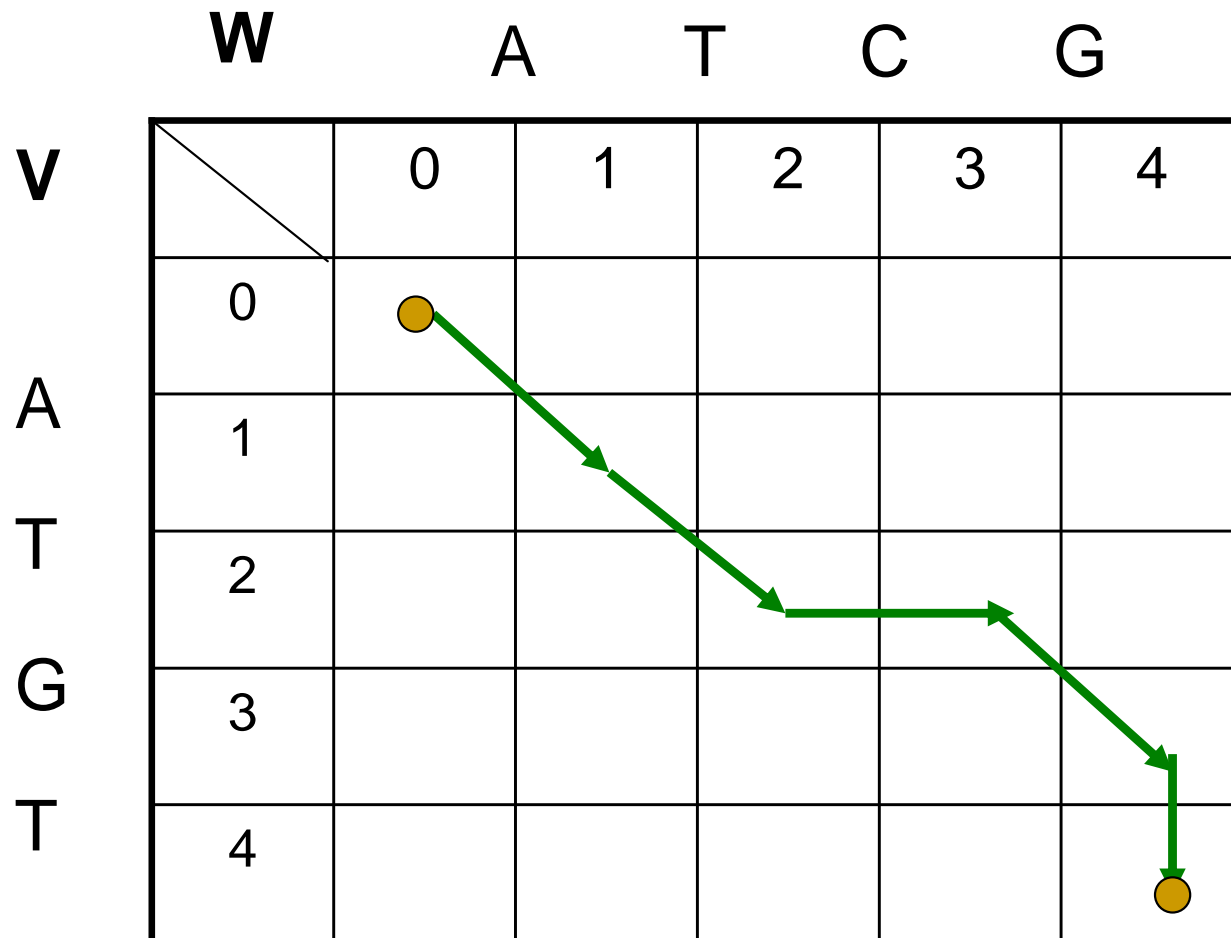
and  $\mathbf{w}_j =$  prefix of  $\mathbf{w}$  of length  $j$ :  $w_1 \dots w_j$

The length of  $\text{LCS}(\mathbf{v}_i, \mathbf{w}_j)$  is computed by:

$$s_{i,j} = \max \begin{cases} s_{i-1,j} \\ s_{i,j-1} \\ s_{i-1,j-1} + 1 \text{ if } v_i = w_j \end{cases}$$



# Every Path in the Grid Corresponds to an Alignment



$\swarrow \swarrow \rightarrow \swarrow \downarrow$   
 0 1 2 2 3 4  
 V = A T - G T  
   | | |  
 W = A T C G -  
   0 1 2 3 4 4



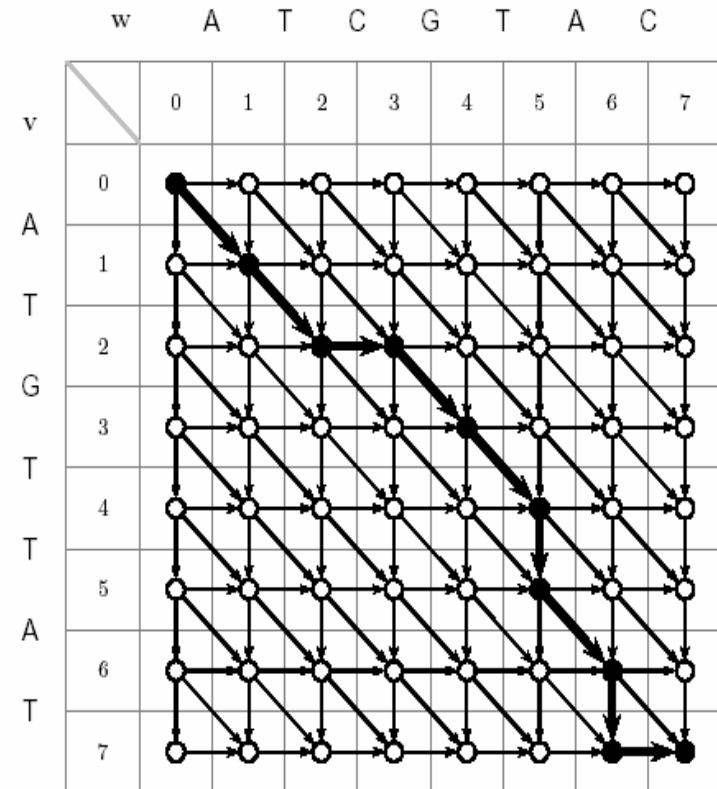
# The Alignment Grid

```

v = 0 1 2 2 3 4 5 6 7 7
 A T - G T T A T -
w = | | | | | | | |
 A T C G T - A - C
 0 1 2 3 4 5 5 6 6 7

```

- Every alignment path is from source to sink

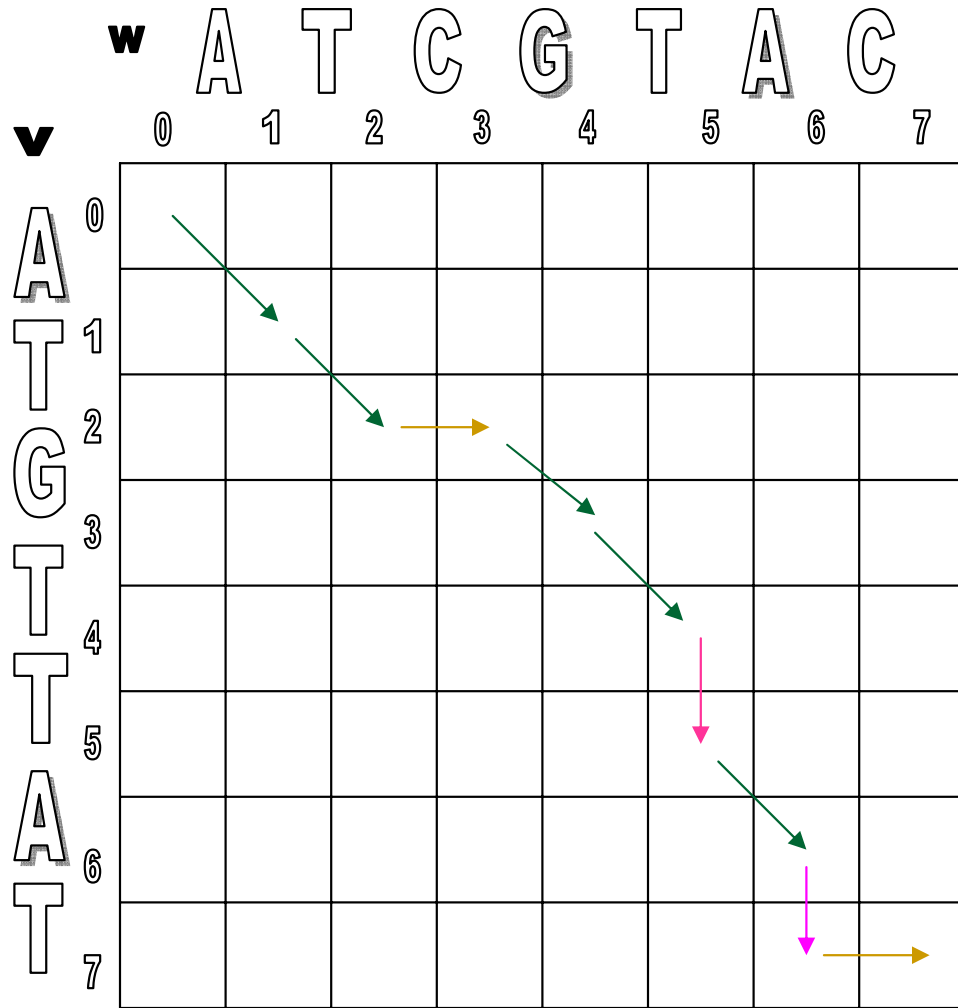


```

 \ \ → \ \ ↓ \ ↓ →
 A T - G T T A T -
 A T C G T - A - C

```

# Alignments in Edit Graph (cont'd)



↓ and → represent indels in **v** and **w** with score 0.

↘ represent matches with score 1.

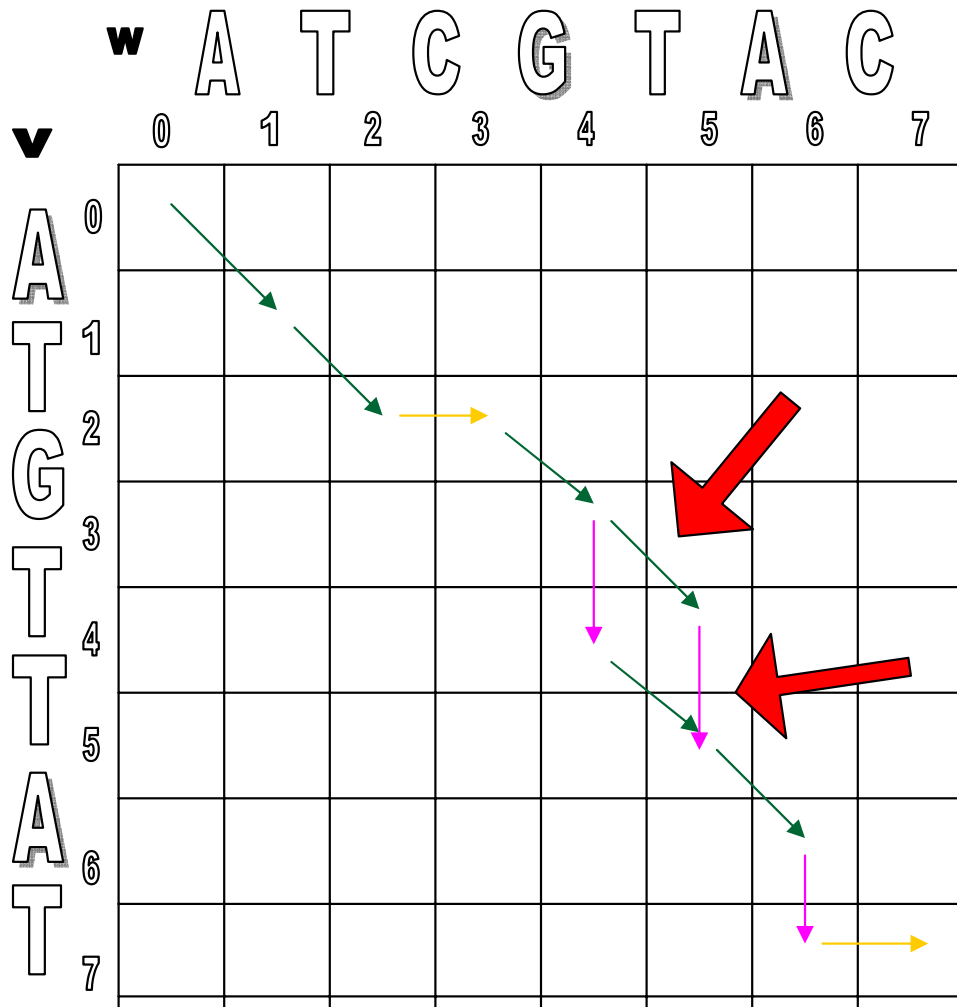
- The score of the alignment path is 5.

Every path in the edit graph corresponds to an alignment:



|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| \ | \ | - | \ | \ |   |   | - |
| A | T | - | G | T | T | A | T |
| A | T | C | G | T | - | A | - |

# Alignment as a Path in the Edit Graph



## Old Alignment

0122345677  
 v= AT\_GTTAT\_  
 w= ATCGT\_A\_C  
 0123455667

## New Alignment

0122345677  
 v= AT\_GTTAT\_  
 w= ATCG\_TA\_C  
 0123445667

# Dynamic Programming Example

|   |   | w | A | T | C | G | T | A | C |   |
|---|---|---|---|---|---|---|---|---|---|---|
|   |   | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |   |
| v | A | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
|   | T | 1 | 0 |   |   |   |   |   |   |   |
|   | G | 2 | 0 |   |   |   |   |   |   |   |
|   | T | 3 | 0 |   |   |   |   |   |   |   |
|   | T | 4 | 0 |   |   |   |   |   |   |   |
|   | A | 5 | 0 |   |   |   |   |   |   |   |
|   | A | 6 | 0 |   |   |   |   |   |   |   |
|   | T | 7 | 0 |   |   |   |   |   |   |   |


Initialize  $1^{st}$  row and  $1^{st}$  column to be all zeroes.

Or, to be more precise, initialize  $0^{th}$  row and  $0^{th}$  column to be all zeroes.

# Dynamic Programming Example


|   |   | w |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
|   |   | A | T | C | G | T | A | C |   |
|   |   | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| v | A | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
|   | T | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
|   | G | 0 | 1 |   |   |   |   |   |   |
|   | T | 0 | 1 |   |   |   |   |   |   |
|   | T | 0 | 1 |   |   |   |   |   |   |
|   | T | 0 | 1 |   |   |   |   |   |   |
|   | A | 0 | 1 |   |   |   |   |   |   |
|   | T | 0 | 1 |   |   |   |   |   |   |

$$S_{i,j} = \max \begin{cases} S_{i-1,j-1} & \leftarrow \text{value from NW} + 1, \text{ if } v_i = w_j \\ S_{i-1,j} & \leftarrow \text{value from North (top)} \\ S_{i,j-1} & \leftarrow \text{value from West (left)} \end{cases}$$

Arrows  show where the score originated from.

 if from the top

 if from the left

 if  $v_i = w_j$

# Backtracking Example

|   | w | A | T | C | G | T | A | C |
|---|---|---|---|---|---|---|---|---|
| v | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| A | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| T | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| G | 0 | 1 | 2 | 2 | 2 | 2 | 2 | 2 |
| T | 0 | 1 | 2 |   |   |   |   |   |
| T | 0 | 1 | 2 |   |   |   |   |   |
| T | 0 | 1 | 2 |   |   |   |   |   |
| A | 0 | 1 | 2 |   |   |   |   |   |
| T | 0 | 1 | 2 |   |   |   |   |   |

Find a match in row and column 2.

$i=2, j=2,5$  is a match (T).

$j=2, i=4,5,7$  is a match (T).

Since  $v_i = w_j$ ,  $s_{i,j} = s_{i-1,j-1} + 1$

$$s_{2,2} = [s_{1,1} = 1] + 1$$

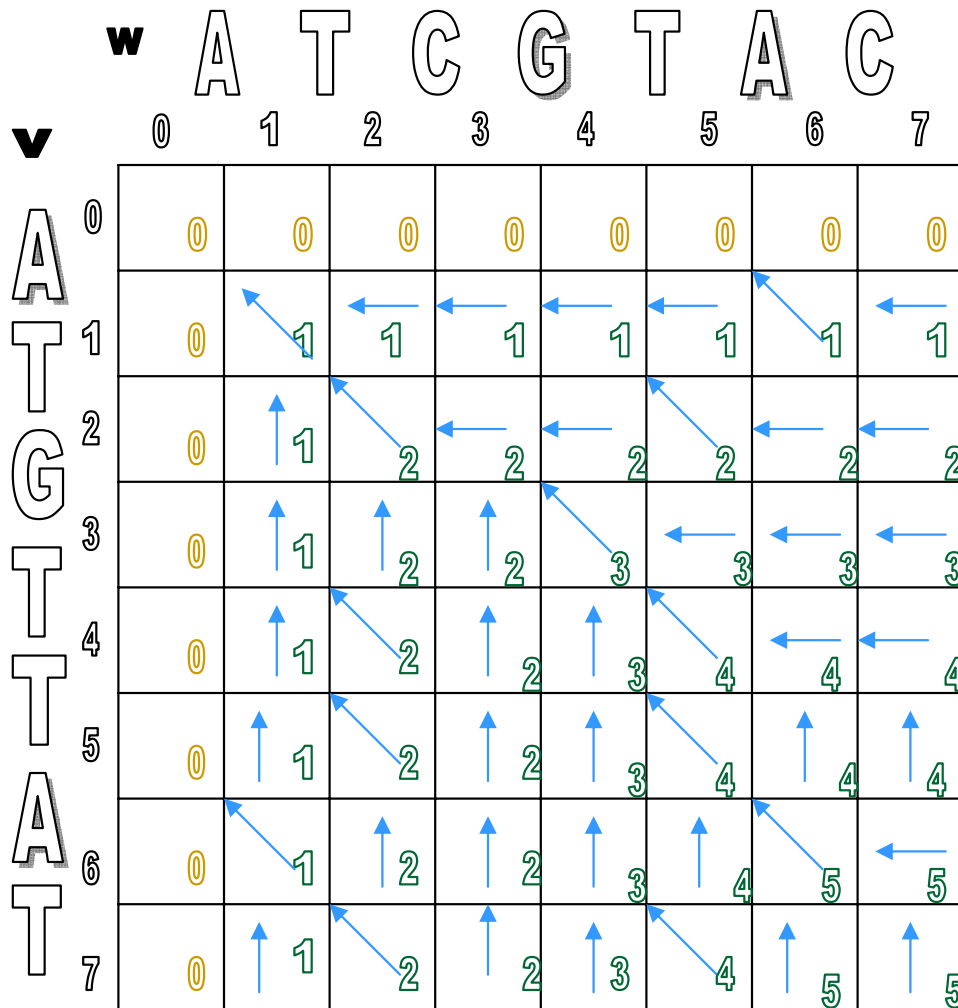
$$s_{2,5} = [s_{1,4} = 1] + 1$$

$$s_{4,2} = [s_{3,1} = 1] + 1$$

$$s_{5,2} = [s_{4,1} = 1] + 1$$

$$s_{7,2} = [s_{6,1} = 1] + 1$$

# Backtracking Example



Continuing with the dynamic programming algorithm gives this result.

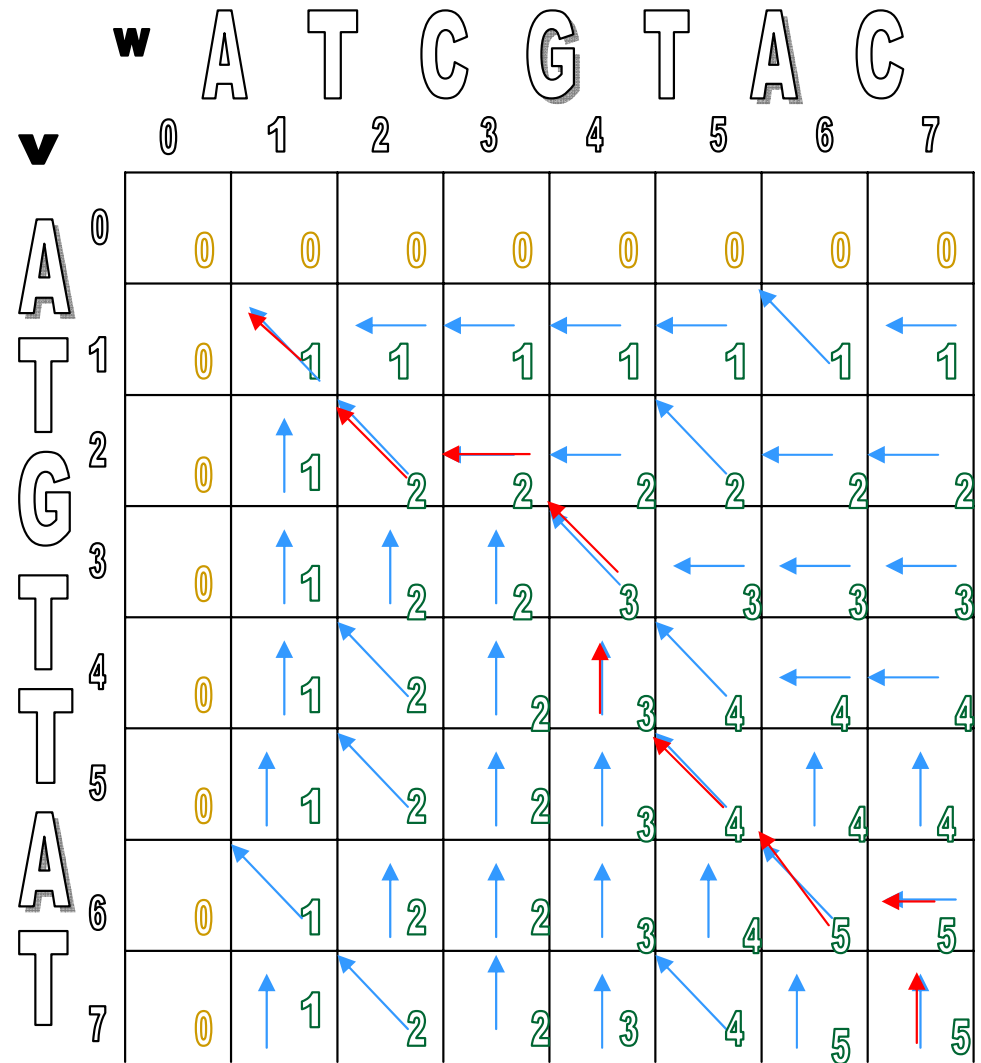
# LCS Algorithm

```
1. LCS(v, w)
2. for $i = 1$ to n
3. $s_{i,0} = 0$
4. for $j = 1$ to m
5. $s_{0,j} = 0$
6. for $i = 1$ to n
7. for $j = 1$ to m
8. $s_{i,j} = \max \begin{cases} s_{i-1,j} \\ s_{i,j-1} \\ s_{i-1,j-1} + 1, \text{ if } v_i = w_j \end{cases}$
9. $b_{i,j} = \begin{cases} \uparrow & \text{if } s_{i,j} = s_{i-1,j} \\ \leftarrow & \text{if } s_{i,j} = s_{i,j-1} \\ \swarrow & \text{if } s_{i,j} = s_{i-1,j-1} + 1 \end{cases}$
10.
11.
■ return $(s_{n,m}, b)$
```



# Now What?

- $LCS(v,w)$  created the alignment grid
- Now we need a way to read the best alignment of  $v$  and  $w$
- Follow the arrows backwards from sink



# Printing LCS: Backtracking

1. **PrintLCS(b,v,i,j)**
  2.     **if**  $i = 0$  or  $j = 0$
  3.         **return**
  4.     **if**  $b_{i,j} = \nwarrow$
  5.         **PrintLCS(b,v,i-1,j-1)**
  6.         **print**  $v_i$
  7.     **else**
  8.         **if**  $b_{i,j} = \uparrow$
  9.             **PrintLCS(b,v,i-1,j)**
  10.         **else**
  11.             **PrintLCS(b,v,i,j-1)**
-

---

# LCS Runtime

- It takes  $O(nm)$  time to fill in the  $n \times m$  dynamic programming matrix.
  - Why  $O(nm)$ ? The pseudocode consists of a nested “for” loop inside of another “for” loop to set up a  $n \times m$  matrix.
-

---

# Summary

- The running times of algorithms is important!
    - If it doesn't scale up, it won't be useful, especially in bioinformatics
  - Recursion is a basic technique which is useful for breaking down problems into simpler ones
  - Dynamic programming, which uses recursion, is often used in bioinformatics as well
    - Shown to be mathematically accurate
    - However, it can be inefficient for more than two sequences
      - BLAST and FASTA use heuristics (human-like techniques to speed up the computations)
-