COL 351 : Analysis & Design of Algorithms

LECTURE 26

DYNAMIC PROGRAMMING IV :

SEQUENCE ALIGNMENT (CONTD.) & BELLMAN FORD ALGORITHM

OCT 04, 2024 | ROHIT VAISH

SEQUENCE ALIGNMENT

input : strings $X = x_1 x_2 \cdots x_m$ $Y = y_1 y_2 \cdots y_n$ over alphabet Σ

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a way of inserting gaps into one or both strings so that they have equal length

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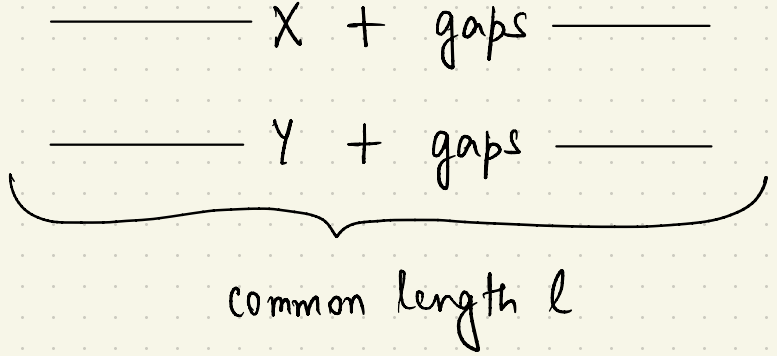
alignment: a way of inserting gaps into one or both strings so that they have equal length



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a way of inserting gaps into one or both strings so that they have equal length

——— X + gaps ———

——— Y + gaps ———

common length l

e.g.,

O_currance

OCCurrence

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$$X = A\ G\ G\ C\ T$$

$$Y = A\ C\ G\ G\ C\ C$$

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$$X = A\ G\ G\ C\ T$$

$$Y = A\ C\ G\ G\ C\ C$$

Which is better:

$$\begin{matrix} A & G & G & C & T & \_ \\ A & C & G & G & C & C \end{matrix} \quad \text{or} \quad \begin{matrix} A & \_ & G & G & C & \_ & T \\ A & C & G & G & C & C & \_ \end{matrix} \quad ?$$

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input : strings $X = x_1 x_2 \cdots x_m$ $Y = y_1 y_2 \cdots y_n$ over alphabet Σ

output : an alignment of X and Y with minimum total penalty.

Gap penalty α_{gap}

Mismatch penalty α_{xy}

where $x, y \in \Sigma$

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input: strings $X = x_1 x_2 \cdots x_m$ $Y = y_1 y_2 \cdots y_n$ over alphabet Σ

output: an alignment of X and Y with minimum total penalty.

Gap penalty $\alpha_{gap} \geq 0$ Why?

Mismatch penalty α_{xy}

where $x, y \in \Sigma$

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c _ a _ t

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Sum of all gap and mismatch penalties

Needleman - Wunsch (NW) score

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Example: $\alpha_{gap} = 1$ $\alpha_{xy} = 2$ $\forall x, y \in \Sigma$

$X = A\ G\ T\ A\ C\ G$

$Y = A\ C\ A\ T\ A\ G$

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NW score = ?

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No gaps $\Rightarrow$ penalty = 8

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$X =$ A G T A C G

$Y =$ A C A T A G

A _ _ G T A C G

A C A _ T A _ G

Four gaps $\Rightarrow$ penalty $= 4$

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output: an alignment of X and Y with minimum total penalty.

Example: $\alpha_{gap} = 1$ $\alpha_{xy} = 2$ $\forall x, y \in \Sigma$

Is penalty ≤ 3 possible?

$X =$ A G T A C G

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Is penalty ≤ 3 possible? No!

Strings of equal length $\Rightarrow$ #gaps is even

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If # gaps $= 0$, then # mismatches $= 4$

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If # gaps $= 4$, then penalty ≥ 4

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Is penalty ≤ 3 possible? No!

Strings of equal length $\Rightarrow$ # gaps is even

If # gaps $= 0$, then # mismatches $= 4$

If # gaps $= 4$, then penalty ≥ 4

If # gaps $= 2$, then # mismatches ≥ 1.

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NW score = 4.

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output: an alignment of X and Y with minimum total penalty.

(Exercise)

alignments between X and Y: exponential in $(n + m)$.

Brute force is prohibitive ☹️

OPTIMAL SUBSTRUCTURE

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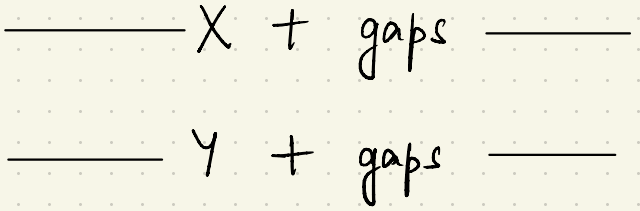
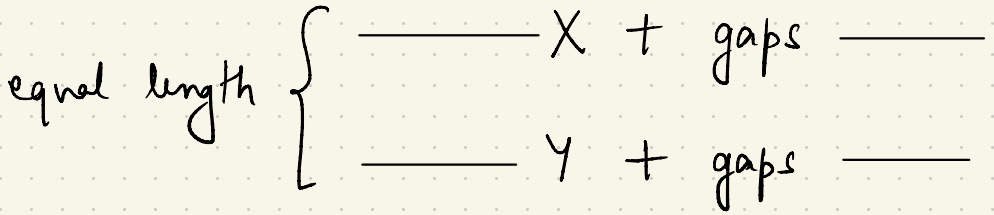


OPTIMAL SUBSTRUCTURE



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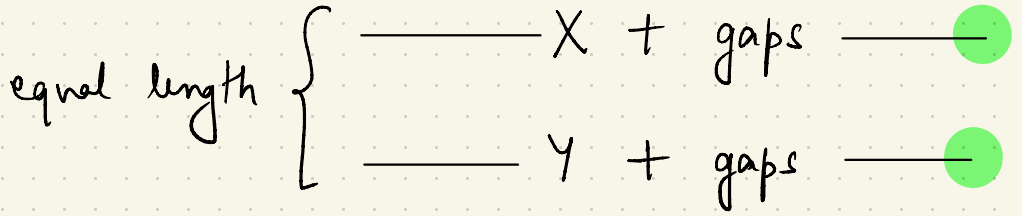
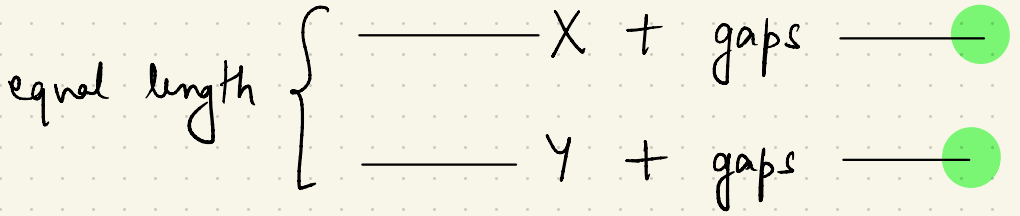


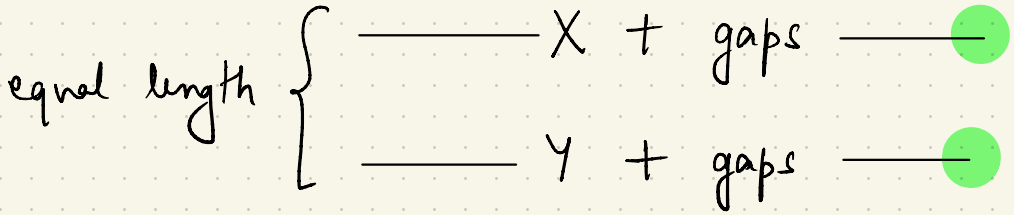
OPTIMAL SUBSTRUCTURE

How many relevant cases ?



OPTIMAL SUBSTRUCTURE

How many relevant cases ? Three



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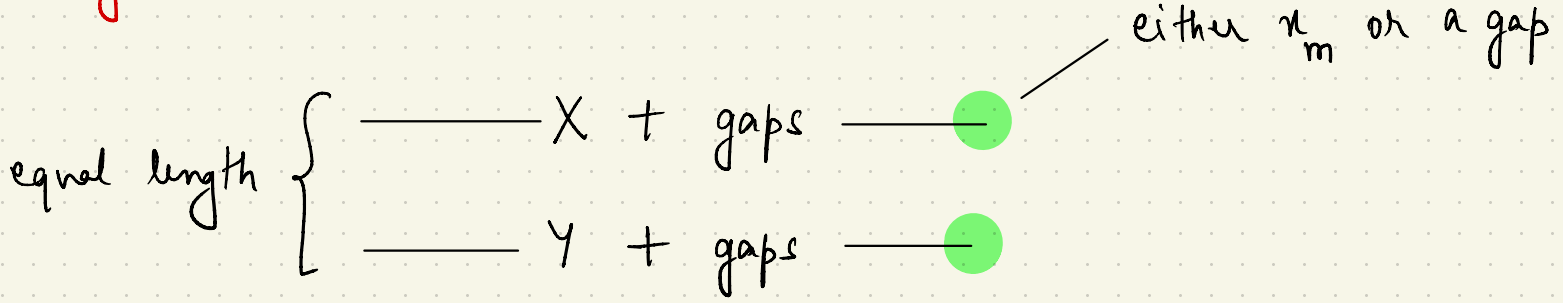

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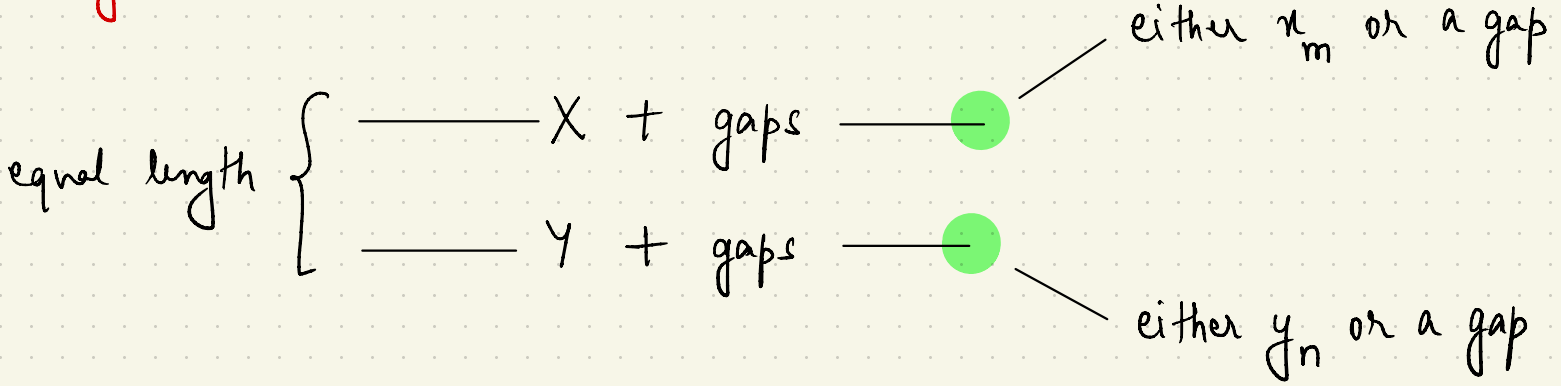

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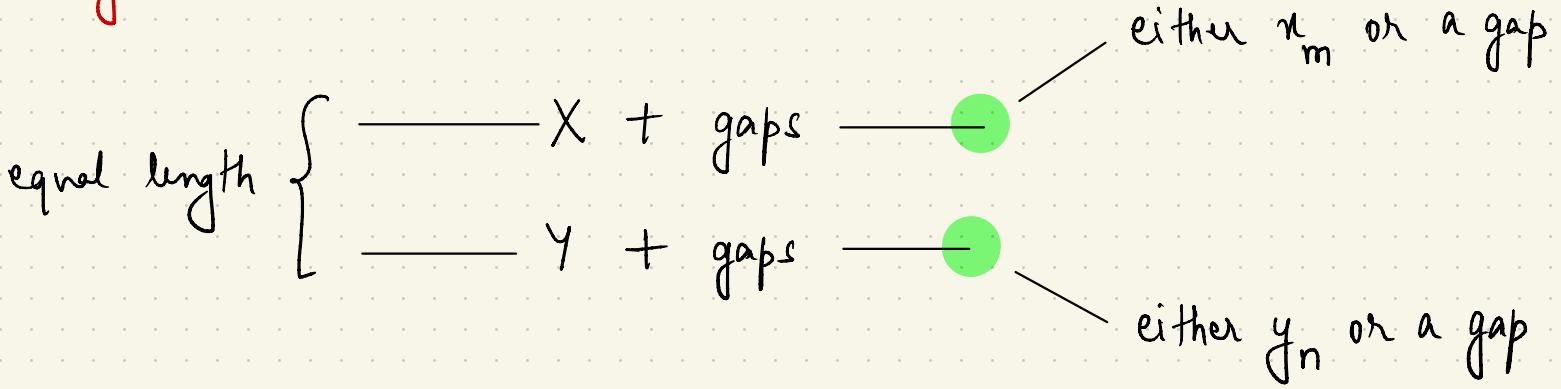
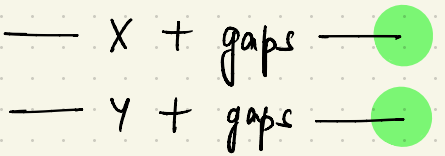


$\alpha_{gap} \geq 0 \Rightarrow$ both can't be gaps !

OPTIMAL SUBSTRUCTURE



OPTIMAL SUBSTRUCTURE

Let $X' := X - x_m$ $\quad Y' := Y - y_n$

— X + gaps —

— Y + gaps —

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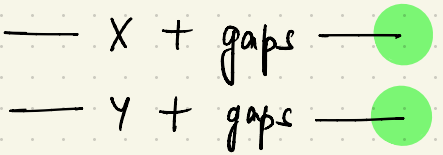

Case I: Final characters are x_m and y_n

Case II: Final characters are x_m and gap

Case III: Final characters are gap and y_n

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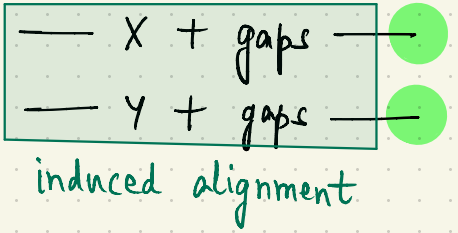

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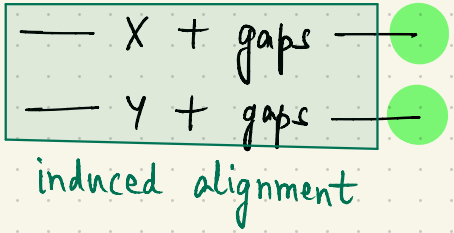

Case I: Final characters are x_m and y_n

$\Rightarrow$ induced alignment of X' and Y' is optimal.

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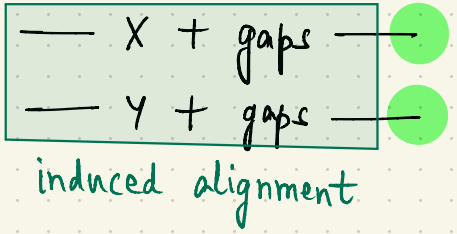

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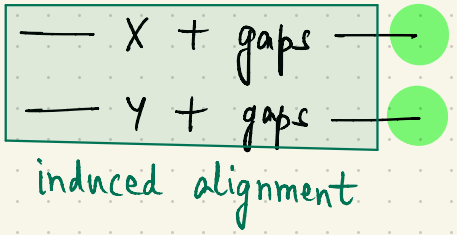

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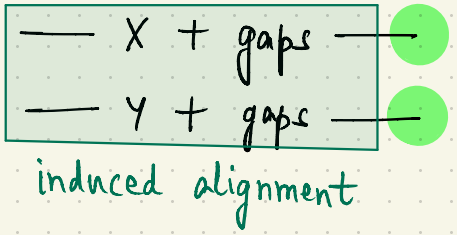

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Case III : Final characters are gap and y_n

$\Rightarrow$ induced alignment of X and Y' is optimal.

Exercise : Prove formally.

Relevant Subproblems

Subproblems are two-dimensional (like knapsack)

X_i := first i letters of X

Y_j := first j letters of Y

The Recurrence

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Define $P_{i,j}$:= penalty of optimal alignment of X_i and Y_j

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THE RECURRENCE

Define $P_{i,j}$:= penalty of optimal alignment of X_i and Y_j

For all $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$

$P_{i,j} =$

// case I

// case II

// case III

The Recurrence

Define $P_{i,j}$:= penalty of optimal alignment of X_i and Y_j

For all $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$

$$P_{i,j} = \begin{cases} \alpha_{x_i y_j} + P_{(i-1),(j-1)} & \text{// case I} \\ & \text{// case II} \\ & \text{// case III} \end{cases}$$

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Base cases: $P_{i,0} := ?$

The Recurrence

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Base cases: $P_{i,0} := i \cdot \alpha_{gap}$

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Base cases: $P_{i,0} := i \cdot \alpha_{gap}$ $\quad P_{0,j} := j \cdot \alpha_{gap}$

THE ALGORITHM

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A = two-dimensional array of size $(m+1) \times (n+1)$

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// base cases

$A[i, 0] = i \cdot \alpha_{gap} \quad \forall\ i$

$A[0, j] = j \cdot \alpha_{gap} \quad \forall\ j$

THE ALGORITHM

A = two-dimensional array of size $(m+1) \times (n+1)$

// base cases

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$A[0,j] = j \cdot \alpha_{gap} \quad \forall\ j$

// main loop

for $i = 1, 2, \cdots, m$

    for $j = 1, 2, \cdots, n$

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for $i = 1, 2, \cdots, m$

  for $j = 1, 2, \cdots, n$

$$A[i,j] = \min \begin{cases} A[i-1, j-1] + \alpha_{x_i, y_j} \\ A[i-1, j] + \alpha_{gap} \\ A[i, j-1] + \alpha_{gap} \end{cases}$$

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Reconstruction : Easy Case I, II, III explicitly tells us where a gap is inserted.

REVISITING SINGLE SOURCE SHORTEST PATHS

SINGLE-SOURCE SHORTEST PATH PROBLEM

input: A directed graph $G = (V, E)$, starting vertex s, a non negative length l_e for each edge $e \in E$

output: dist (s, v) for every vertex $v \in V$.

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length of the shortest path from s to v if $s \rightsquigarrow v$ path exists

∞ otherwise

ON DIJKSTRA'S ALGORITHM

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Solution: Bellman-Ford algorithm

NEGATIVE CYCLES

How to define shortest paths in the presence of negative cycles?

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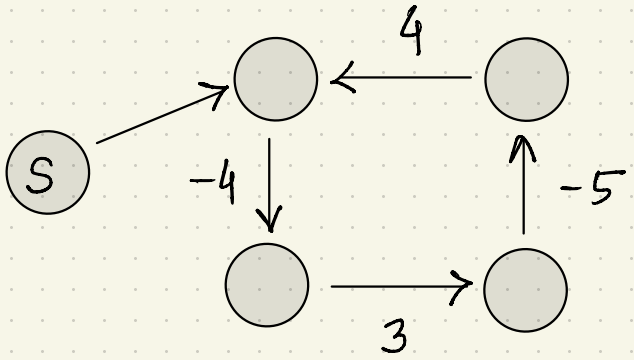

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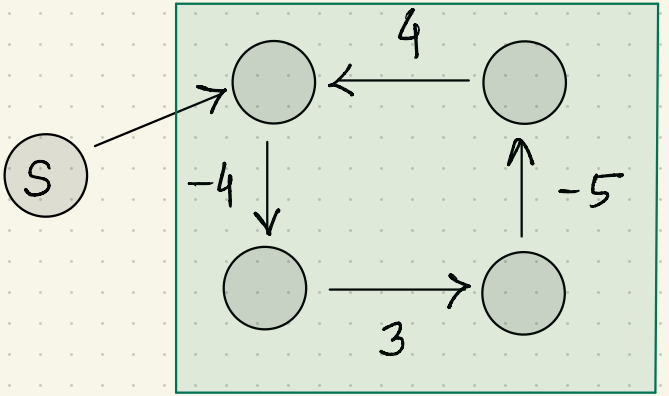

cycle with weight -2

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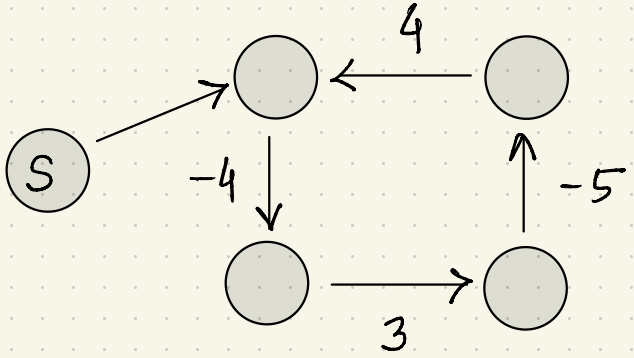

If we include cycles in shortest paths

then length of the shortest path is undefined (or $-\infty$).

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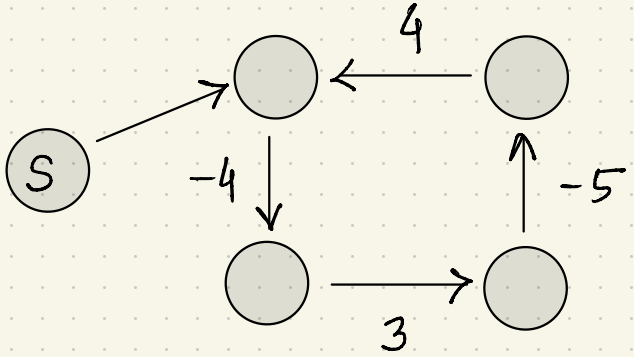

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then the problem is NP-complete (no known poly-time algo.)

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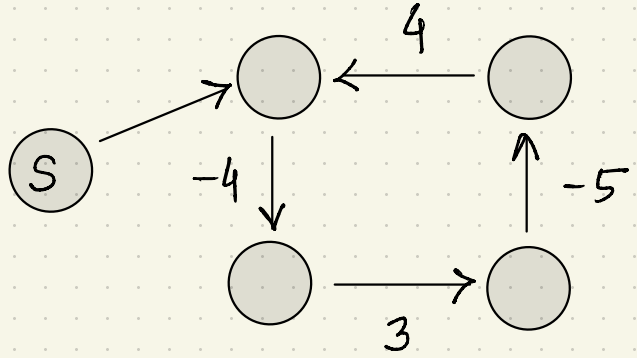

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encodes "longest path" problem

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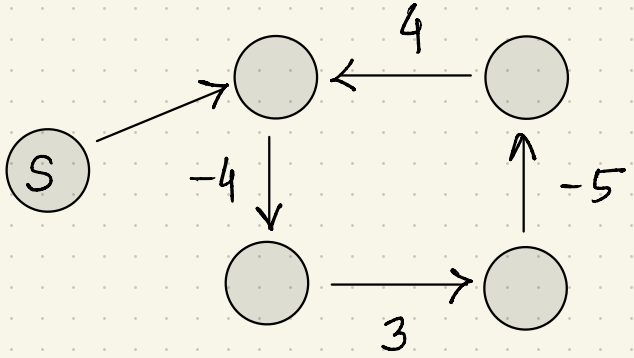

Solution: Allow negative length edges but not negative cycles.

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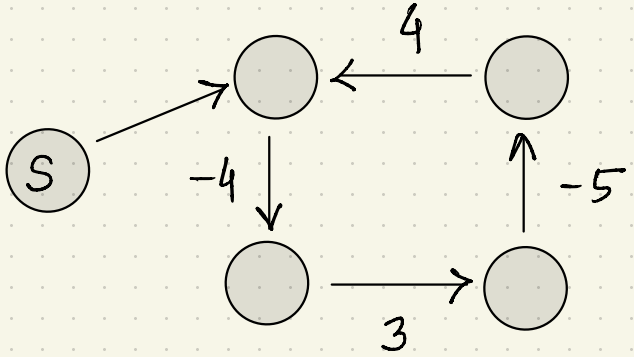

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Will show how to quickly check this