# CS 580: Algorithm Design and Analysis

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**Announcement:** Homework 3 due February 15th at 11:59PM
**Midterm Exam:** Wed, Feb 21 (8PM-10PM) @ MTHW 210

# Recap: Dynamic Programming

**Key Idea: Express optimal solution in terms of solutions to smaller sub problems**

**Example 1**: Knapsack Problem

- **Two Dimensional Solution OPT(j,w)**
- **$OPT(j,w) = \max\{ v_j + OPT(w-w_j), OPT(j-1,w)\}$**
- Case 1: Optimal solution includes item j with value $v_j$
  - Add item j and reduce remaining capacity to $w-w_j$
- Case 2: Optimal solution does not include item j

**Example 2:** RNA Secondary Structure

- **Goal:** Maximize number of matched base pairs
- **Constraints:** No Sharp Turns, Watson-Crick Complements, No Crossing Edges
- $OPT(i, j)$ = maximum number of base pairs in a secondary structure of the substring $b_i b_{i+1} \ldots b_j$
- $OPT(i, j) = \mathbf{max}\{Opt(i,j-1), \mathbf{max}_t \{1+OPT(i,t-1) + OPT(t+1,j-1)\} \}$

# 6.6 Sequence Alignment

# String Similarity

How similar are two strings?

- ocurrance
- occurrence

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| o | c | u | r | r | a | n | c | e | - |
| o | c | c | u | r | r | e | n | c | e |

6 mismatches, 1 gap

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| o | c | - | u | r | r | a | n | c | e |
| o | c | c | u | r | r | e | n | c | e |

1 mismatch, 1 gap

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| o | c | - | u | r | r | - | a | n | c | e |
| o | c | c | u | r | r | e | - | n | c | e |

0 mismatches, 3 gaps

# Edit Distance

**Applications.**

- Basis for Unix diff.
- Speech recognition.
- Computational biology.

**Edit distance.** [Levenshtein 1966, Needleman-Wunsch 1970]

- Gap penalty $\delta$; mismatch penalty $\alpha_{pq}$.
- Cost = sum of gap and mismatch penalties.

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

$\alpha_{TC} + \alpha_{GT} + \alpha_{AG} + 2\alpha_{CA}$

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

$2\delta + \alpha_{CA}$

# Sequence Alignment

**Goal:** Given two strings $X = x_1 x_2 \ldots x_m$ and $Y = y_1 y_2 \ldots y_n$ find alignment of minimum cost.

**Def.** An alignment $M$ is a set of ordered pairs $x_i$-$y_j$ such that each item occurs in at most one pair and no crossings.

**Def.** The pair $x_i$-$y_j$ and $x_{i'}$-$y_{j'}$ cross if $i < i'$, but $j > j'$.

$$\text{cost}(M) = \underbrace{\sum_{(x_i, y_j) \in M} \alpha_{x_i y_j}}_{\text{mismatch}} + \underbrace{\sum_{i \,:\, x_i \text{ unmatched}} \delta + \sum_{j \,:\, y_j \text{ unmatched}} \delta}_{\text{gap}}$$

**Ex:** CTACCG vs. TACATG.

**Sol:** $M = x_2$-$y_1$, $x_3$-$y_2$, $x_4$-$y_3$, $x_5$-$y_4$, $x_6$-$y_6$.

| | | | | | | |
|---|---|---|---|---|---|---|
| $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | | $x_6$ |
| C | T | A | C | C | - | G |
| - | T | A | C | A | T | G |
| | $y_1$ | $y_2$ | $y_3$ | $y_4$ | $y_5$ | $y_6$ |

# Sequence Alignment: Problem Structure

Def. OPT(i, j) = min cost of aligning strings $x_1 x_2 \ldots x_i$ and $y_1 y_2 \ldots y_j$.

- Case 1: OPT matches $x_i$-$y_j$.
  - pay mismatch for $x_i$-$y_j$ + min cost of aligning two strings $x_1 x_2 \ldots x_{i-1}$ and $y_1 y_2 \ldots y_{j-1}$
- Case 2a: OPT leaves $x_i$ unmatched.
  - pay gap for $x_i$ and min cost of aligning $x_1 x_2 \ldots x_{i-1}$ and $y_1 y_2 \ldots y_j$
- Case 2b: OPT leaves $y_j$ unmatched.
  - pay gap for $y_j$ and min cost of aligning $x_1 x_2 \ldots x_i$ and $y_1 y_2 \ldots y_{j-1}$

$$OPT(i,\ j) = \begin{cases} j\delta & \text{if } i = 0 \\ \min \begin{cases} \alpha_{x_i y_j} + OPT(i-1,\ j-1) \\ \delta + OPT(i-1,\ j) \\ \delta + OPT(i,\ j-1) \end{cases} & \text{otherwise} \\ i\delta & \text{if } j = 0 \end{cases}$$

# Sequence Alignment: Algorithm

```
Sequence-Alignment(m, n, x1x2...xm, y1y2...yn, δ, α) {
   for i = 0 to m
      M[i, 0] = iδ
   for j = 0 to n
      M[0, j] = jδ

   for i = 1 to m
      for j = 1 to n
         M[i, j] = min(α[xi, yj] + M[i-1, j-1],
                          δ + M[i-1, j],
                          δ + M[i, j-1])
   return M[m, n]
}
```

Analysis. $\Theta(mn)$ time and space.

English words or sentences: $m, n \le 10$.

Computational biology: $m = n = 100{,}000$. 10 billions ops OK, but 10GB array?

# 6.7 Sequence Alignment in Linear Space

# Sequence Alignment: Linear Space

Q. Can we avoid using quadratic space?

Easy. Optimal value in $O(m + n)$ space and $O(mn)$ time.

- Compute $OPT(i, \cdot)$ from $OPT(i-1, \cdot)$.
- No longer a simple way to recover alignment itself.

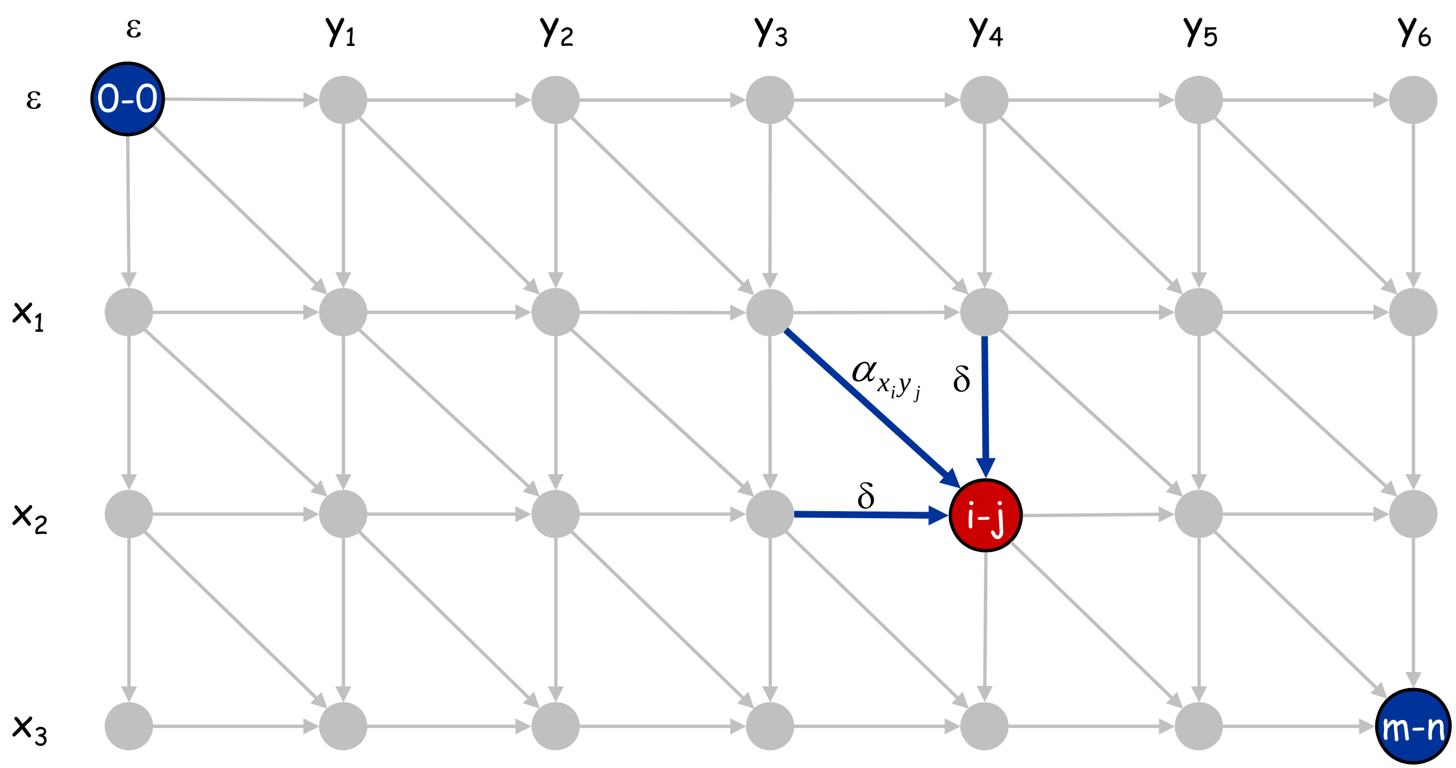
Theorem. [Hirschberg 1975] Optimal alignment in $O(m + n)$ space and $O(mn)$ time.

- Clever combination of divide-and-conquer and dynamic programming.
- Inspired by idea of Savitch from complexity theory.

# Sequence Alignment: Linear Space

Edit distance graph.

- Let f(i, j) be shortest path from (0,0) to (i, j).
- Observation: f(i, j) = OPT(i, j).



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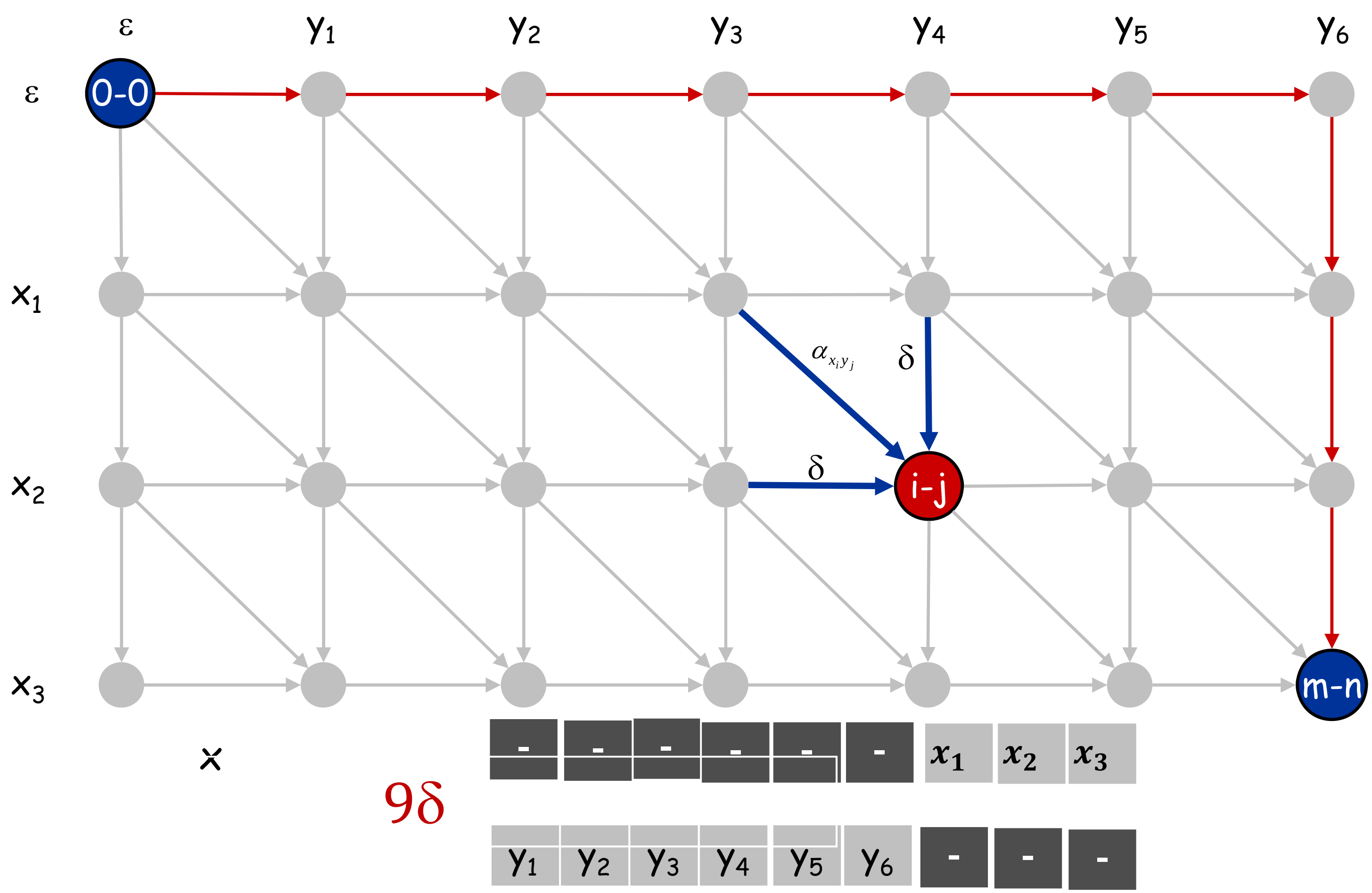

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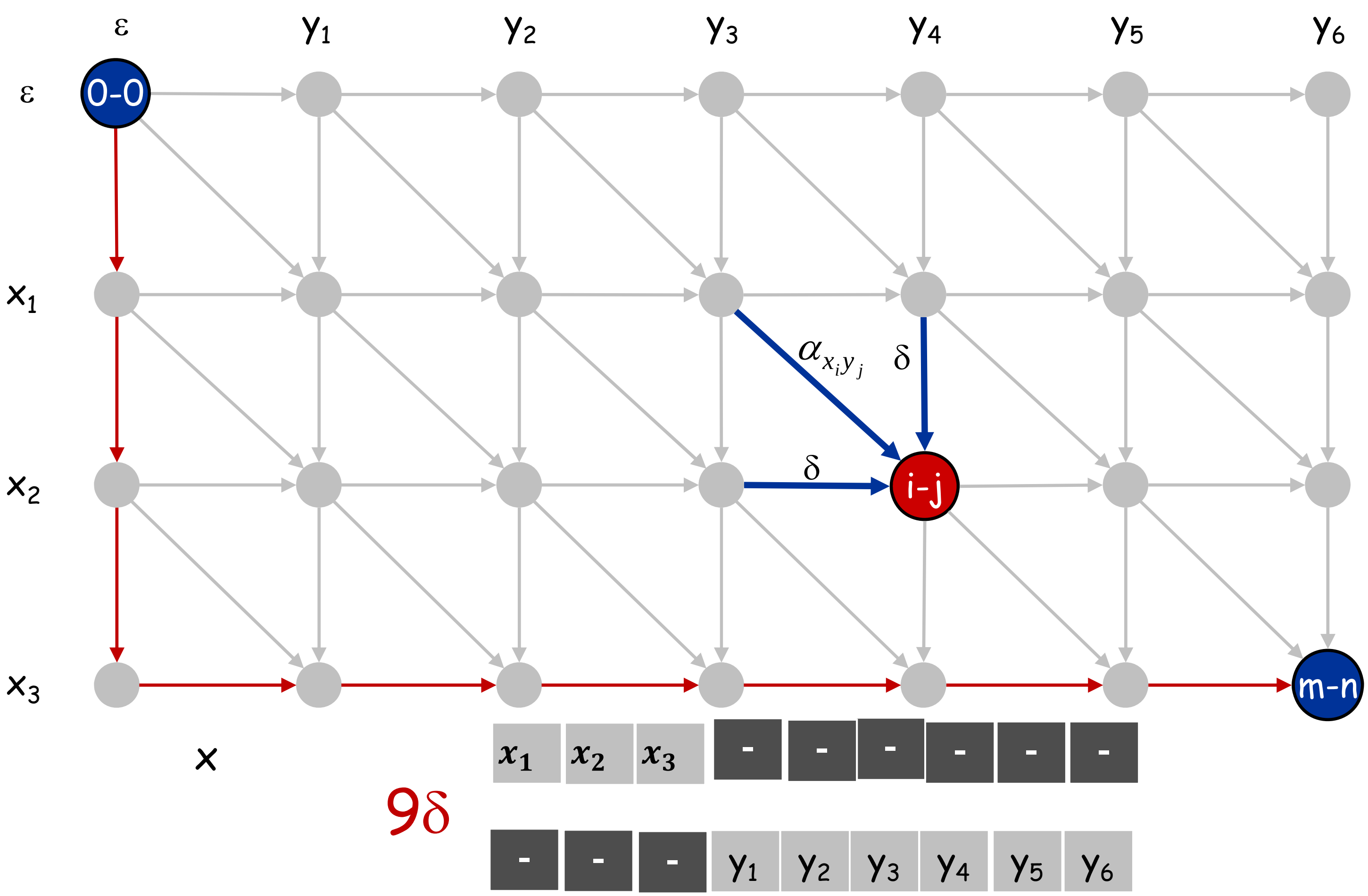

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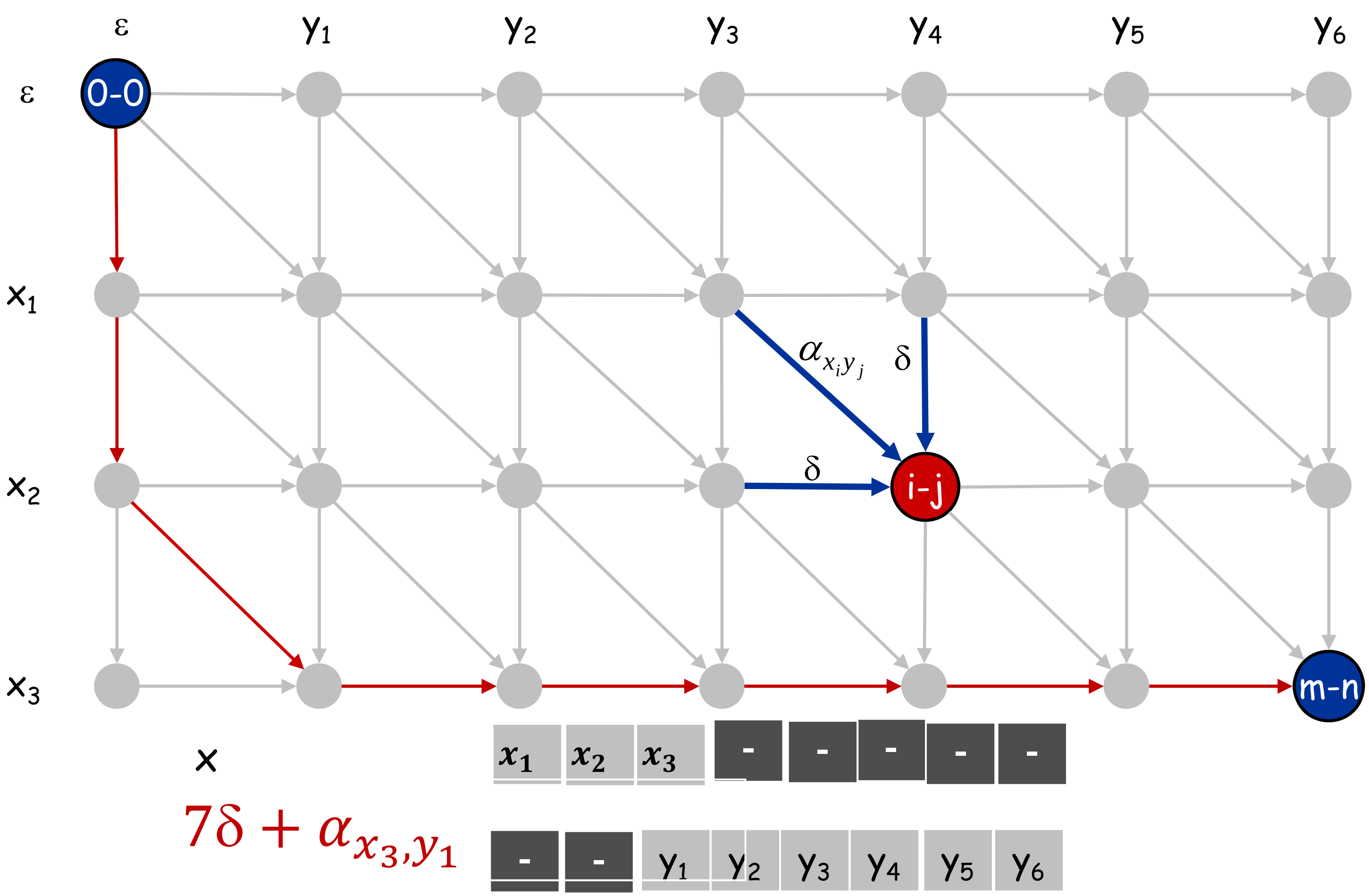
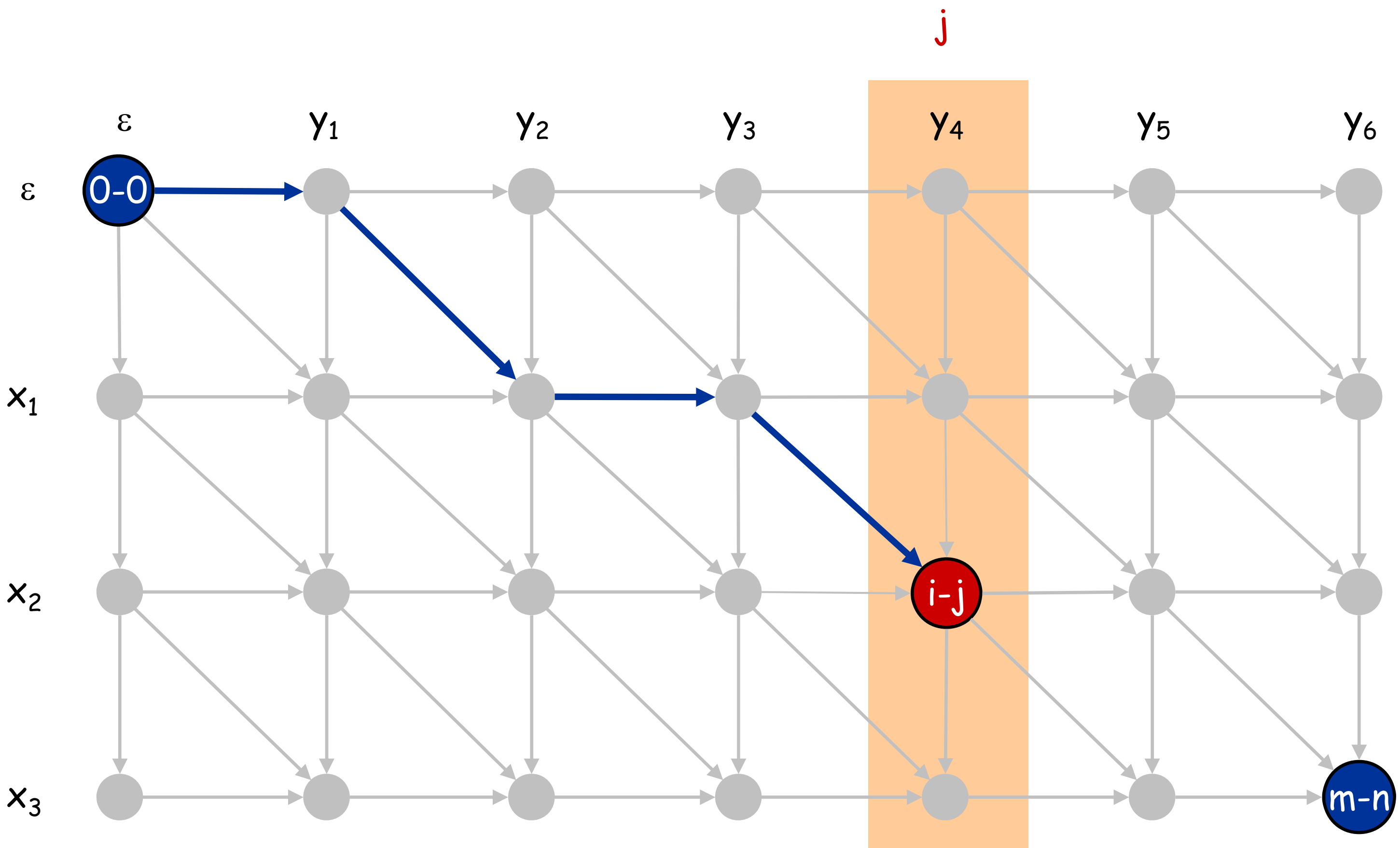


# Sequence Alignment: Linear Space

Edit distance graph.

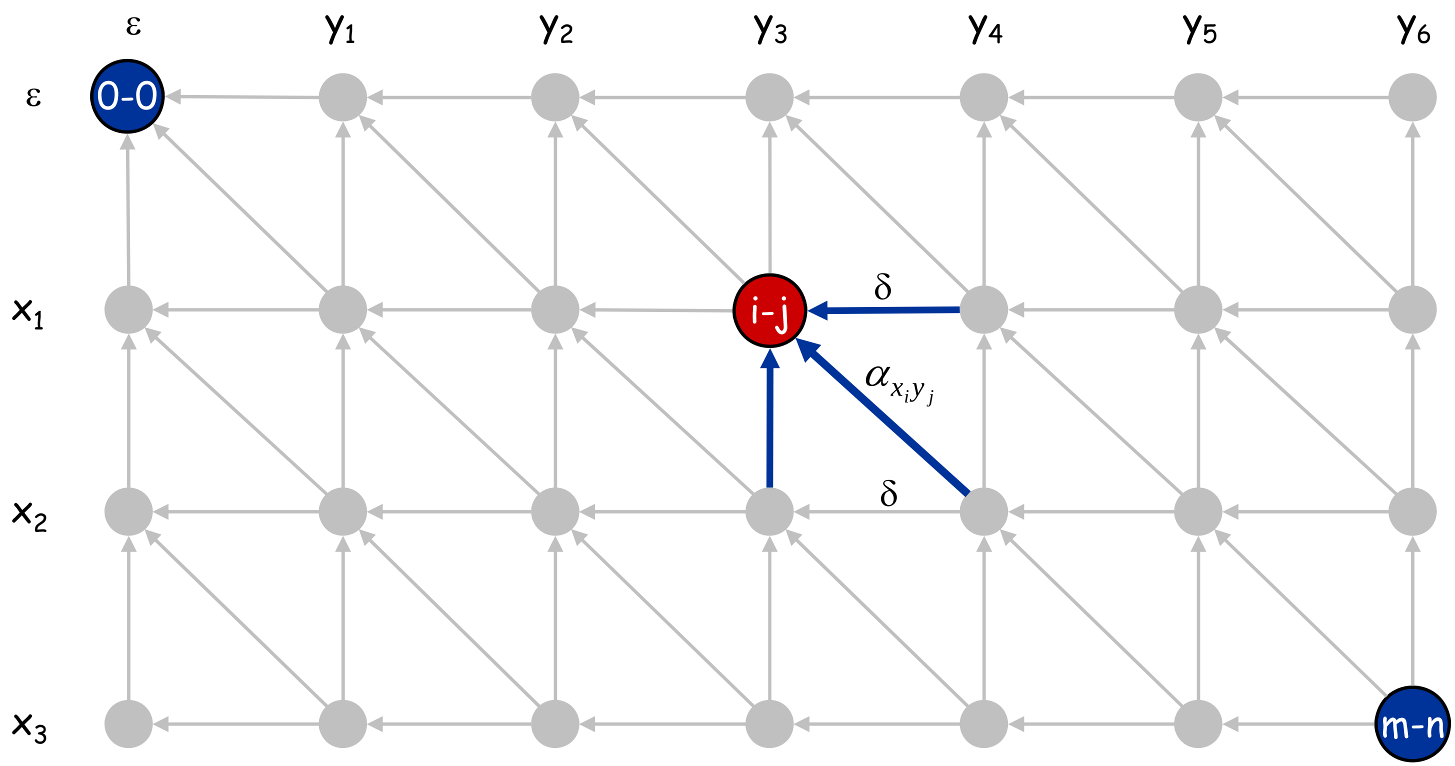
- Let $f(i, j)$ be shortest path from $(0,0)$ to $(i, j)$.
- Can compute $f(\cdot, j)$ for any $j$ in $O(mn)$ time and $O(m + n)$ space.



# Sequence Alignment: Linear Space

Edit distance graph.

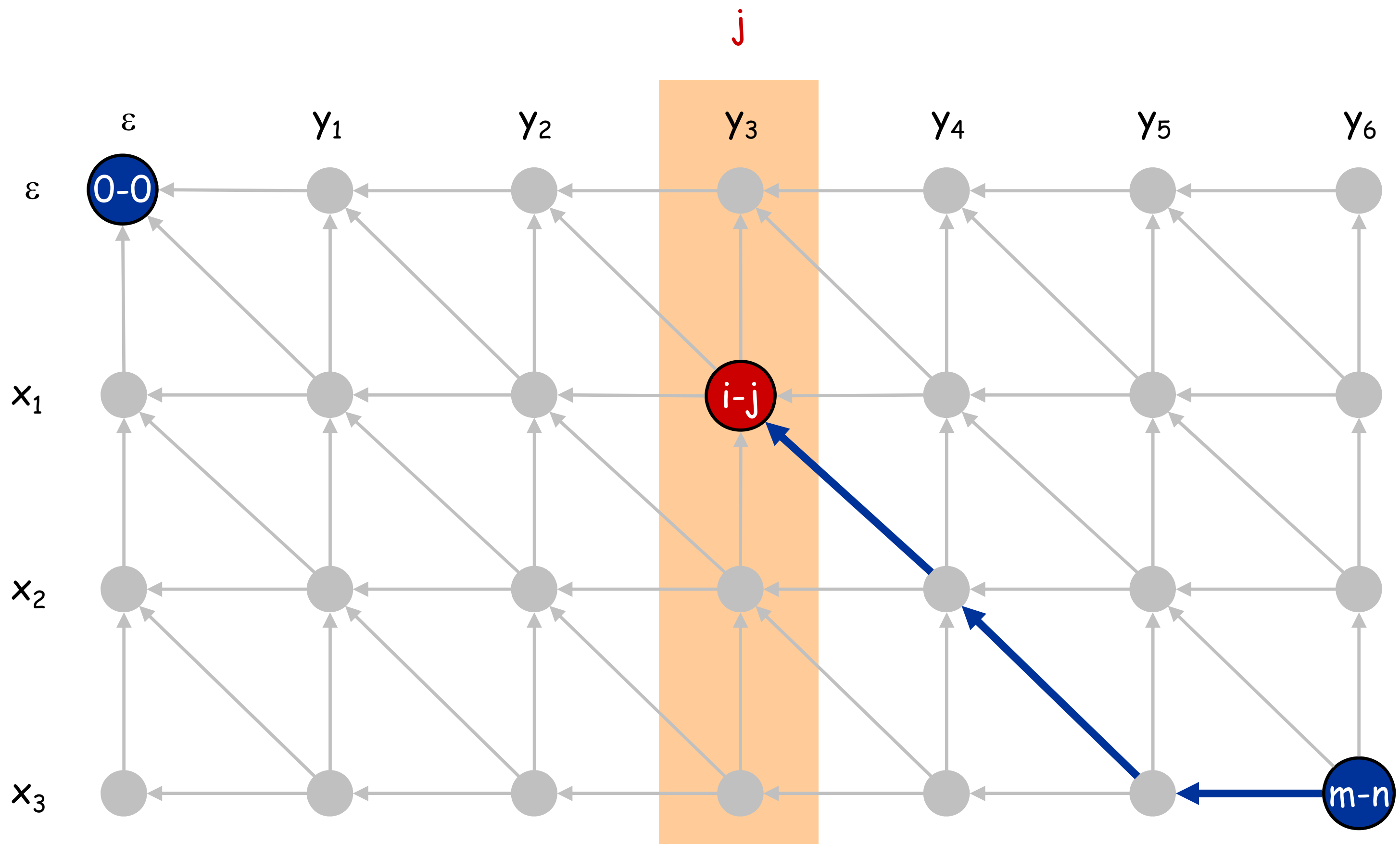
- Let $g(i, j)$ be shortest path from $(i, j)$ to $(m, n)$.
- Can compute by reversing the edge orientations and inverting the roles of $(0, 0)$ and $(m, n)$



# Sequence Alignment: Linear Space

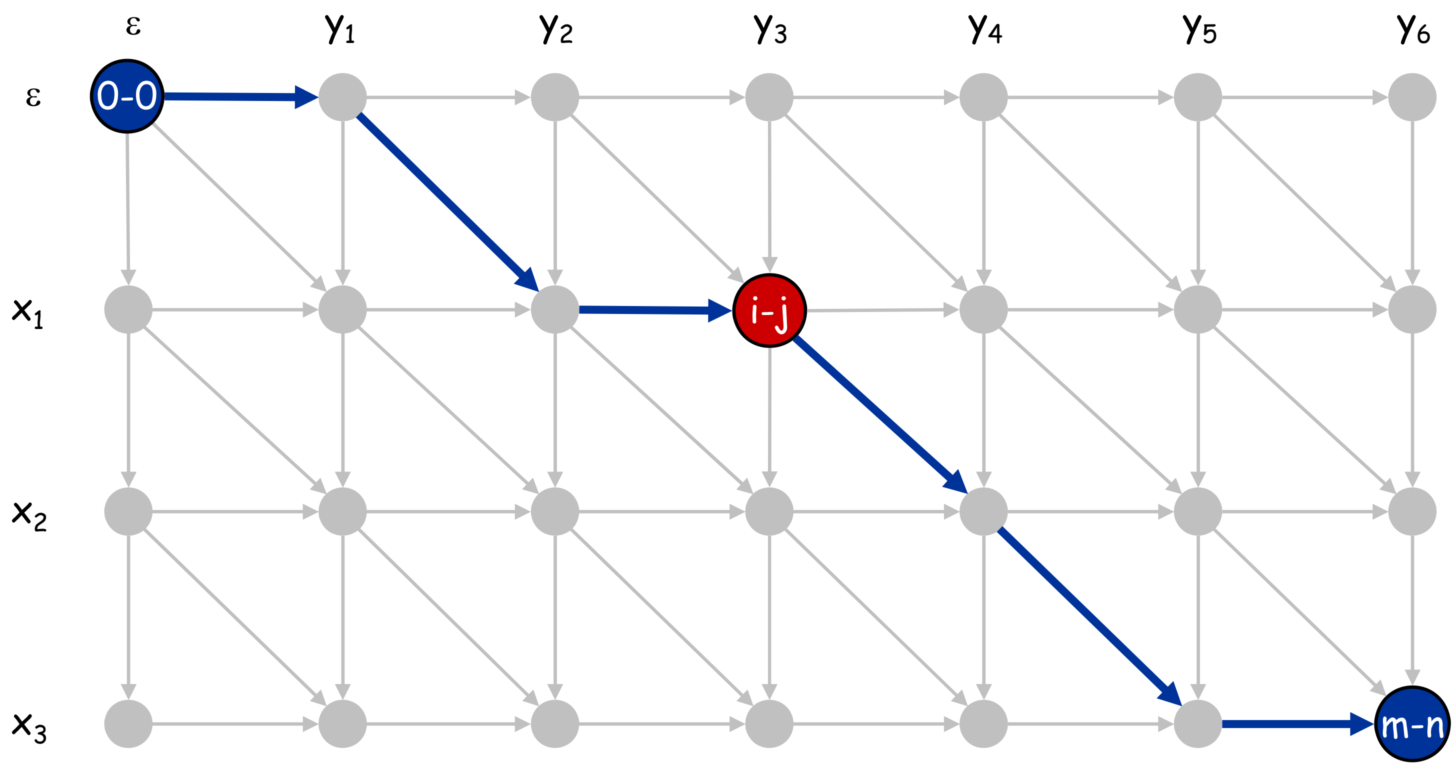
Edit distance graph.

- Let $g(i, j)$ be shortest path from $(i, j)$ to $(m, n)$.
- Can compute $g(\cdot, j)$ for any $j$ in $O(mn)$ time and $O(m + n)$ space.



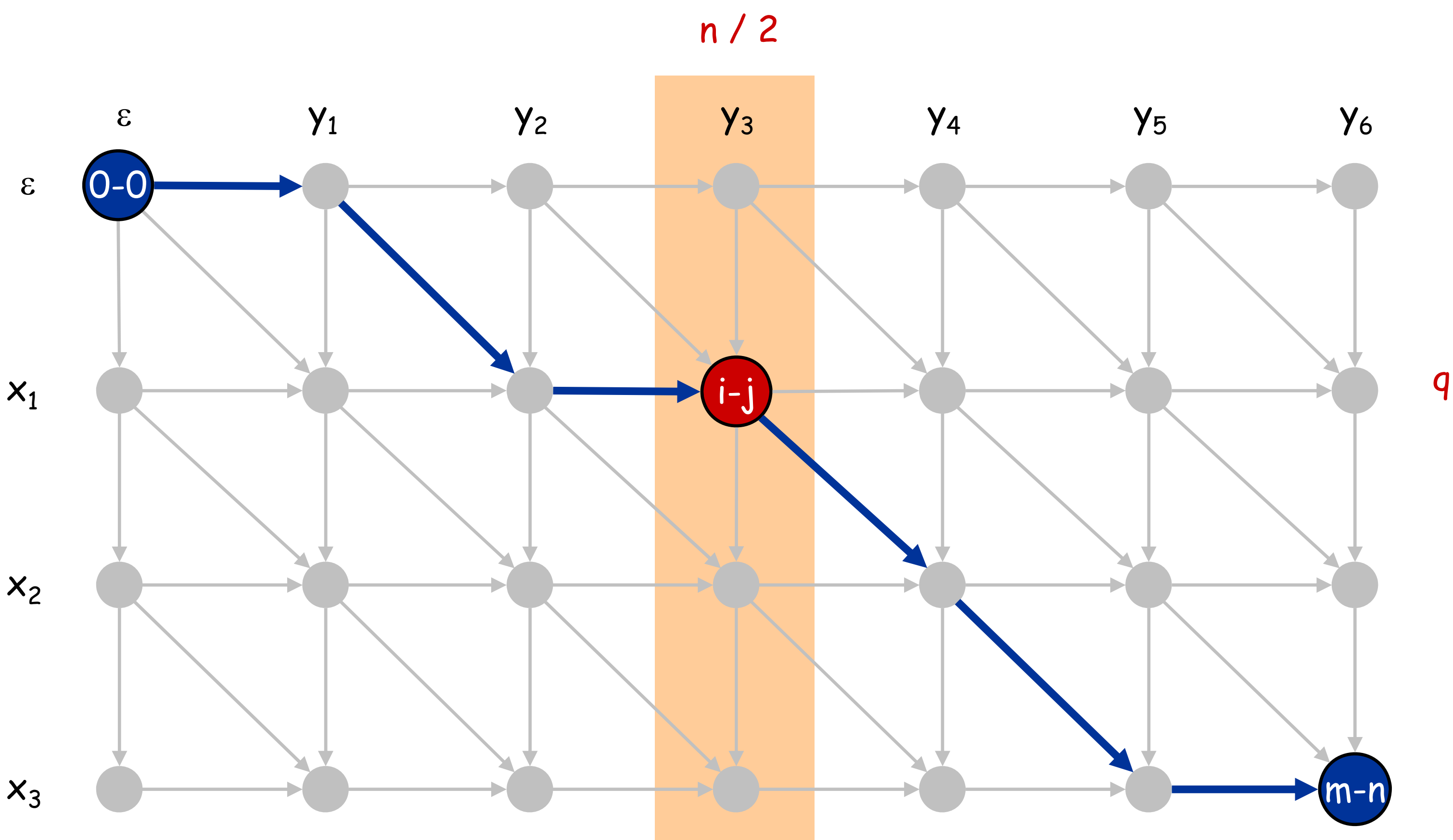
# Sequence Alignment: Linear Space

Observation 1. The cost of the shortest path that uses (i, j) is $f(i, j) + g(i, j)$.



# Sequence Alignment: Linear Space

Observation 2. let q be an index that minimizes f(q, n/2) + g(q, n/2). Then, the shortest path from (0, 0) to (m, n) uses (q, n/2).

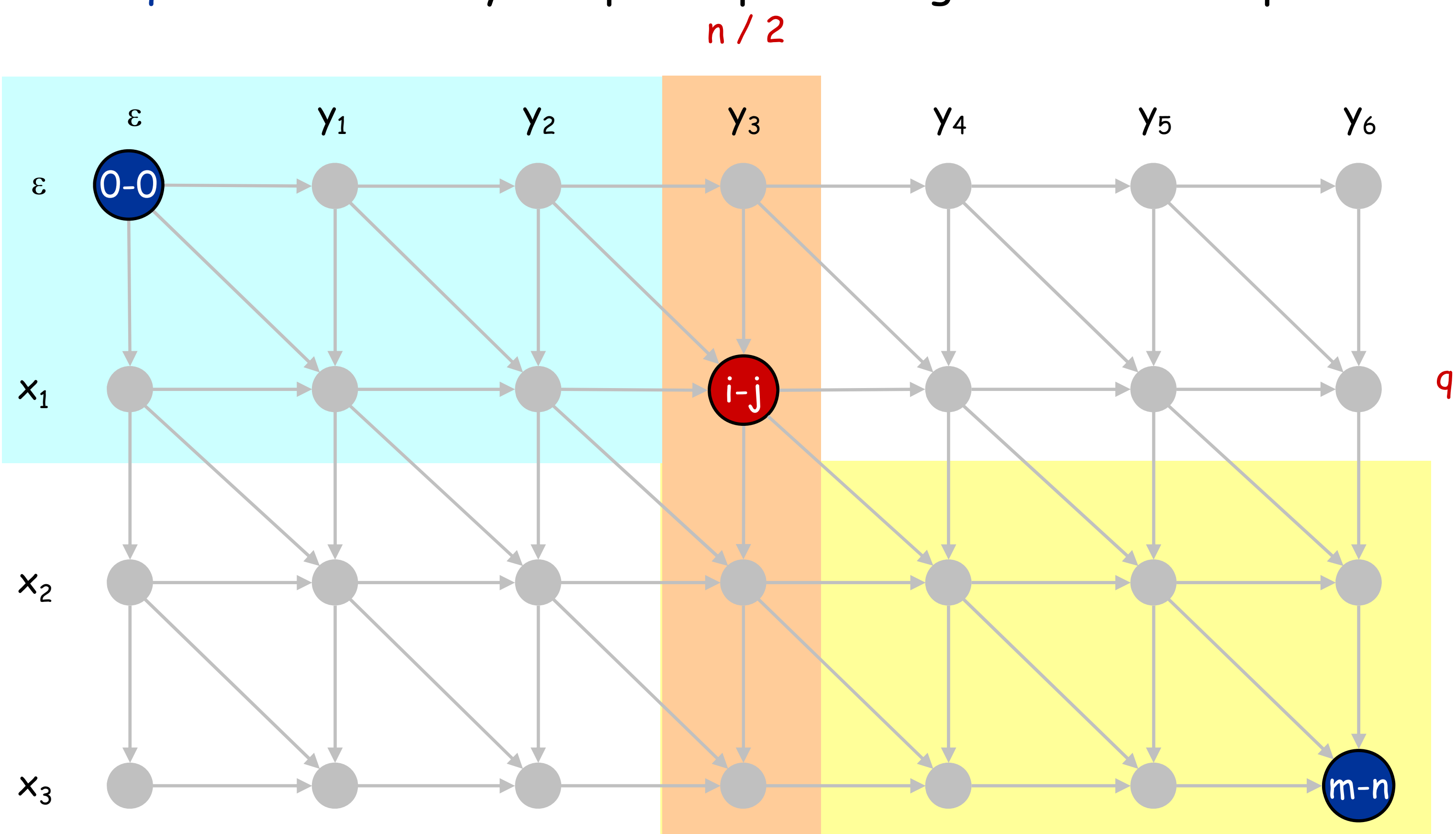


# Sequence Alignment: Linear Space

Divide: find index q that minimizes f(q, n/2) + g(q, n/2) using DP.

- Align $x_q$ and $y_{n/2}$.

Conquer: recursively compute optimal alignment in each piece.



# Sequence Alignment: Running Time Analysis Warmup

Theorem. Let T(m, n) = max running time of algorithm on strings of length at most m and n. T(m, n) = O(mn log n).

$$T(m,n) \leq 2T(m,\ n/2) + O(mn) \quad \Rightarrow \quad T(m,n) = O(mn \log n)$$

Remark. Analysis is not tight because two sub-problems are of size (q, n/2) and (m - q, n/2). In next slide, we save log n factor.

# Sequence Alignment: Running Time Analysis

Theorem. Let T(m, n) = max running time of algorithm on strings of length m and n. T(m, n) = O(mn).

Pf. (by induction on n)

- O(mn) time to compute f( •, n/2) and g ( •, n/2) and find index q.
- T(q, n/2) + T(m - q, n/2) time for two recursive calls.
- Choose constant c so that:

$$\begin{array}{lcl} T(m,\ 2) & \leq & cm \\ T(2,\ n) & \leq & cn \\ T(m,\ n) & \leq & cmn + T(q,\ n/2) + T(m-q,\ n/2) \end{array}$$

- Base cases: m = 2 or n = 2.
- Inductive hypothesis: $T(m, n) \leq 2cmn$.

$$\begin{array}{rcl} T(m,n) & \leq & T(q,n/2) + T(m-q,n/2) + cmn \\ & \leq & 2cqn/2 + 2c(m-q)n/2 + cmn \\ & = & cqn + cmn - cqn + cmn \\ & = & 2cmn \end{array}$$

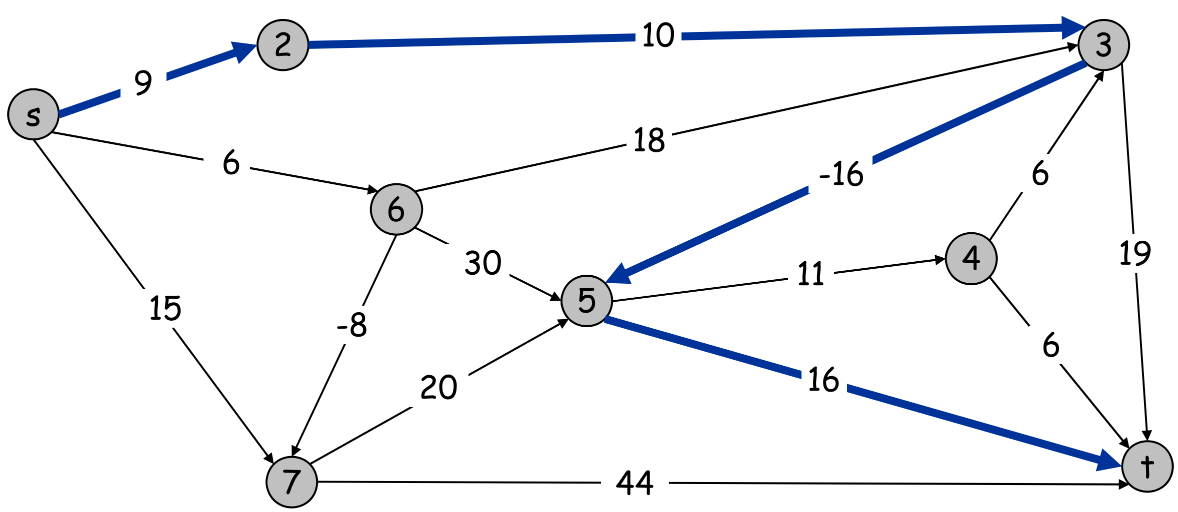
# 6.8 Shortest Paths

# Shortest Paths

Shortest path problem. Given a directed graph $G = (V, E)$, with edge weights $c_{vw}$, find shortest path from node s to node t.

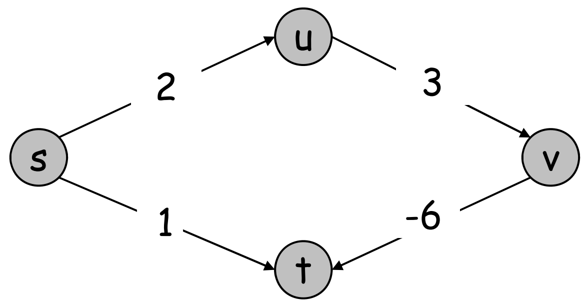
allow negative weights

Ex. Nodes represent agents in a financial setting and $c_{vw}$ is cost of transaction in which we buy from agent v and sell immediately to w.

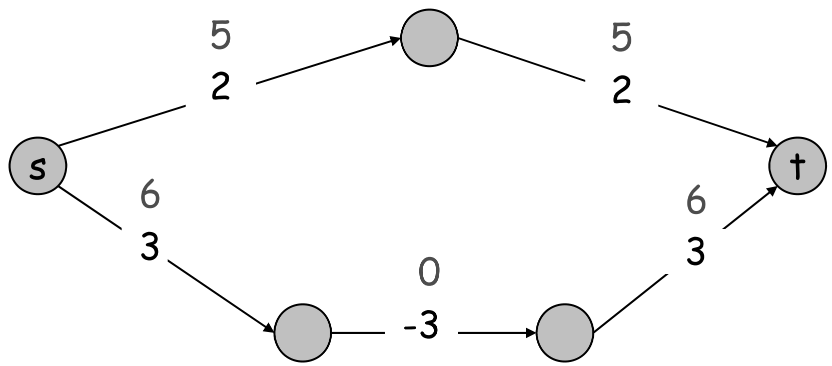


# Shortest Paths: Failed Attempts

Dijkstra. Can fail if negative edge costs.

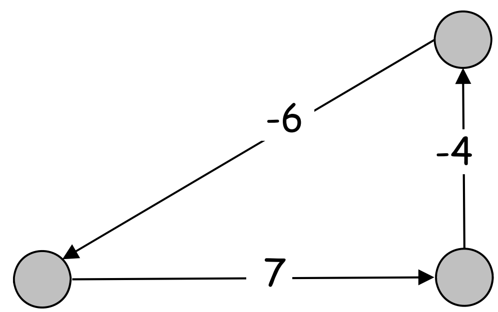



Re-weighting. Adding a constant to every edge weight can fail.

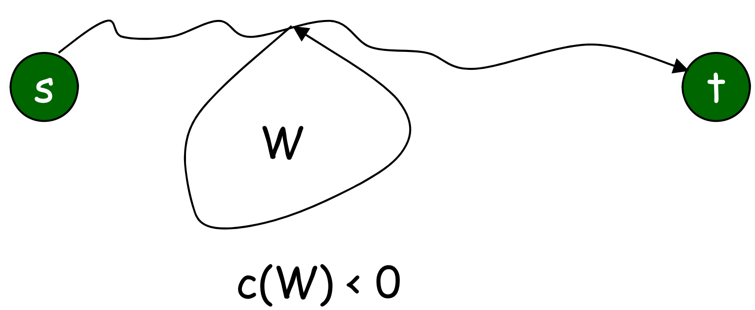


# Shortest Paths: Negative Cost Cycles

Negative cost cycle.




Observation. If some path from s to t contains a negative cost cycle, there does not exist a shortest s-t path; otherwise, there exists one that is simple.



# Shortest Paths: Dynamic Programming

Def. OPT(i, v) = length of shortest v-t path P using at most i edges.

- Case 1: P uses at most i-1 edges.
  - OPT(i, v) = OPT(i-1, v)
- Case 2: P uses exactly i edges.
  - if (v, w) is first edge, then OPT uses (v, w), and then selects best w-t path using at most i-1 edges

$$OPT(i,v) = \begin{cases} 0 & \text{if } i = 0 \\ \min\left\{ OPT(i-1,\ v),\ \min\limits_{(v,w)\in E} \{ OPT(i-1,\ w) + c_{vw} \} \right\} & \text{otherwise} \end{cases}$$

Remark. By previous observation, if no negative cycles, then OPT(n-1, v) = length of shortest v-t path.

# Shortest Paths: Implementation

```
Shortest-Path(G, t) {
   foreach node v ∈ V
      M[0, v] ← ∞
   M[0, t] ← 0

   for i = 1 to n-1
      foreach node v ∈ V
         M[i, v] ← M[i-1, v]
      foreach edge (v, w) ∈ E
         M[i, v] ← min { M[i, v], M[i-1, w] + c_vw }
}
```

Analysis. $\Theta(mn)$ time, $\Theta(n^2)$ space.

Finding the shortest paths. Maintain a "successor" for each table entry.

# Shortest Paths: Practical Improvements

Practical improvements.

- Maintain only one array M[v] = shortest v-t path that we have found so far.
- No need to check edges of the form (v, w) unless M[w] changed in previous iteration.

Theorem. Throughout the algorithm, M[v] is length of some v-t path, and after i rounds of updates, the value M[v] is no larger than the length of shortest v-t path using $\leq$ i edges.

Overall impact.

- Memory: O(m + n).
- Running time: O(mn) worst case, but substantially faster in practice.

# Bellman-Ford: Efficient Implementation

```
Push-Based-Shortest-Path(G, s, t) {
   foreach node v ∈ V {
      M[v] ← ∞
      successor[v] ← φ
   }

   M[t] = 0
   for i = 1 to n-1 {
      foreach node w ∈ V {
      if (M[w] has been updated in previous iteration)
{
         foreach node v such that (v, w) ∈ E {
            if (M[v] > M[w] + c_vw) {
               M[v] ← M[w] + c_vw
               successor[v] ← w
            }
         }
      }
      If no M[w] value changed in iteration i, stop.
   }
}
```

# 6.9 Distance Vector Protocol

# Distance Vector Protocol

Communication network.

- Node ≈ router.
- Edge ≈ direct communication link.
- Cost of edge ≈ delay on link. ← naturally nonnegative, but Bellman-Ford used anyway!

Dijkstra's algorithm. Requires global information of network.

Bellman-Ford. Uses only local knowledge of neighboring nodes.

Synchronization. We don't expect routers to run in lockstep. The order in which each `foreach` loop executes in not important. Moreover, algorithm still converges even if updates are asynchronous.

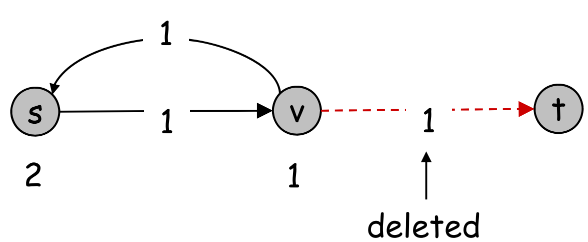
# Distance Vector Protocol

Distance vector protocol.

- Each router maintains a vector of shortest path lengths to every other node (distances) and the first hop on each path (directions).
- Algorithm: each router performs n separate computations, one for each potential destination node.
- "Routing by rumor."

Ex. RIP, Xerox XNS RIP, Novell's IPX RIP, Cisco's IGRP, DEC's DNA Phase IV, AppleTalk's RTMP.

Caveat. Edge costs may change during algorithm (or fail completely).




"counting to infinity"

# Path Vector Protocols

Link state routing.

- Each router also stores the entire path.
- Based on Dijkstra's algorithm.
- Avoids "counting-to-infinity" problem and related difficulties.
- Requires significantly more storage.

not just the distance and first hop

Ex. Border Gateway Protocol (BGP), Open Shortest Path First (OSPF).

# 6.10 Negative Cycles in a Graph

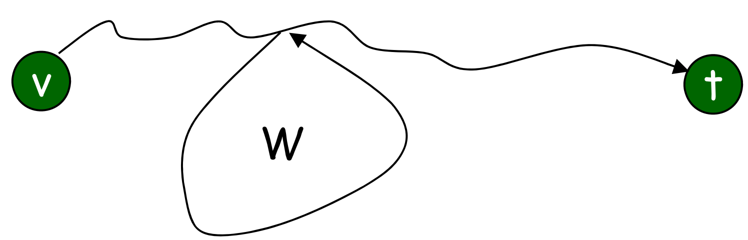
# Detecting Negative Cycles

Lemma. If OPT(n,v) = OPT(n-1,v) for all v, then no negative cycles.
Pf. Bellman-Ford algorithm.

Lemma. If OPT(n,v) < OPT(n-1,v) for some node v, then (any) shortest path from v to t contains a cycle W. Moreover W has negative cost.

Pf. (by contradiction)

- Since OPT(n,v) < OPT(n-1,v), we know P has exactly n edges.
- By pigeonhole principle, P must contain a directed cycle W.
- Deleting W yields a v-t path with < n edges $\Rightarrow$ W has negative cost.

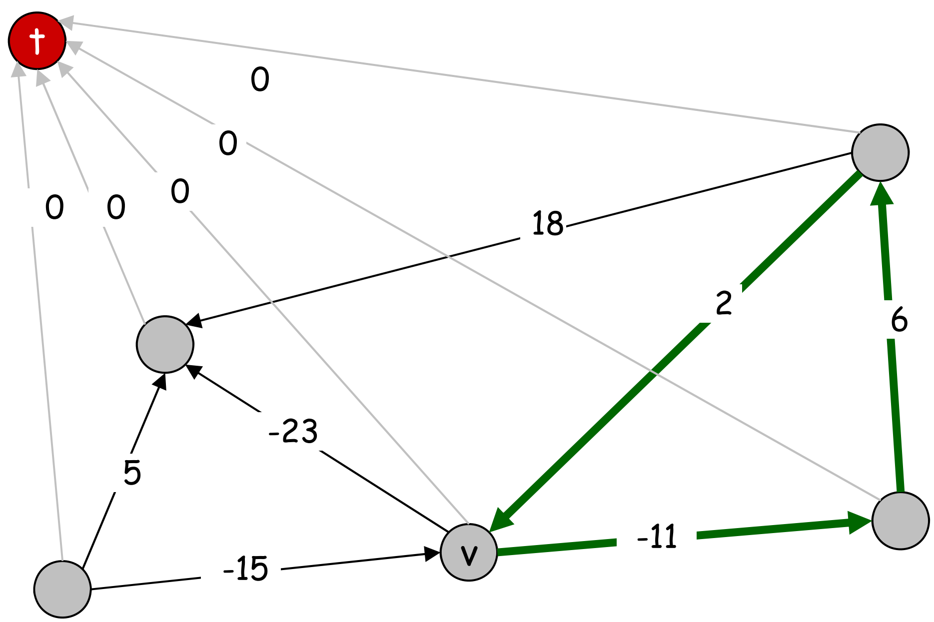



c(W) < 0

# Detecting Negative Cycles

Theorem. Can detect negative cost cycle in O(mn) time.

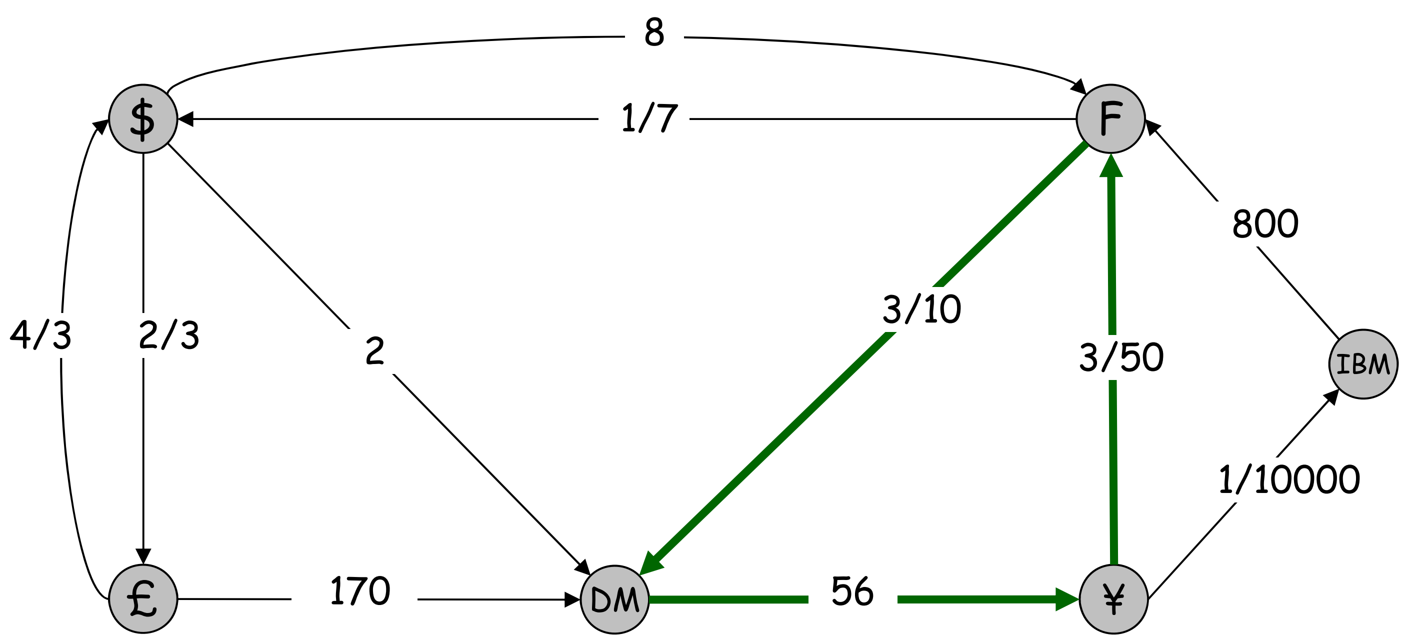
- Add new node t and connect all nodes to t with 0-cost edge.
- Check if OPT(n, v) = OPT(n-1, v) for all nodes v.
  - if yes, then no negative cycles
  - if no, then extract cycle from shortest path from v to t



# Detecting Negative Cycles: Application

Currency conversion. Given n currencies and exchange rates between pairs of currencies, is there an arbitrage opportunity?

Remark. Fastest algorithm very valuable!



# Detecting Negative Cycles: Summary

Bellman-Ford. $O(mn)$ time, $O(m + n)$ space.

- Run Bellman-Ford for n iterations (instead of n-1).
- Upon termination, Bellman-Ford successor variables trace a negative cycle if one exists.
- See p. 304 for improved version and early termination rule.