Divide and Conquer

Outline

- · Overview
- · Weighted Interval Scheduling
- Segmented Least Squares
- · Knapsack Problem
- · RNA Secondary Structure
- · Sequence Alignment
- Shortest Paths with negative weights

Algorithmic Paradigms

Greedy. Build up a solution incrementally, myopically optimizing some local criterion.

Divide-and-conquer. Break up a problem into sub-problems, solve each sub-problem independently, and combine solution to sub-problems to form solution to original problem.

Dynamic programming. Break up a problem into a series of overlapping sub-problems, and build up solutions to larger and larger sub-problems.

Bellman. [1950s] Pioneered the systematic study of dynamic programming.

Dynamic Programming Applications

Areas.

- Bioinformatics.
- Control theory.
- Information theory.
- Operations research.
- Computer science: theory, graphics, AI, compilers, systems,

Some famous dynamic programming algorithms.

- Unix diff for comparing two files.
- Viterbi for hidden Markov models.
- Smith-Waterman for genetic sequence alignment.
- Bellman-Ford for shortest path routing in networks.
- Cocke-Kasami-Younger for parsing context free grammars.

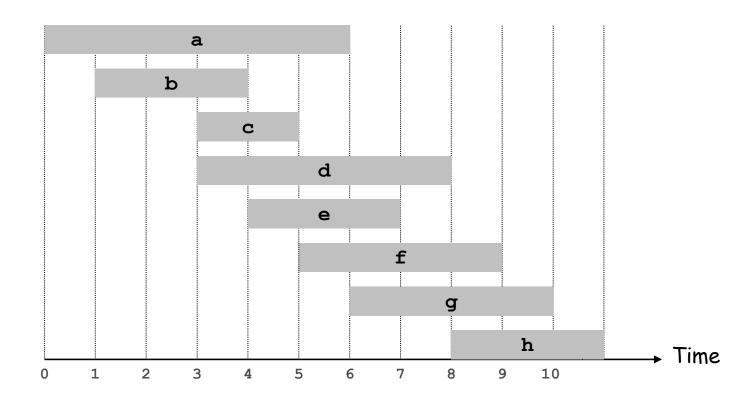
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Weighted Interval Scheduling

Weighted interval scheduling problem.

- \blacksquare Job j starts at s_j , finishes at f_j , and has weight or value v_j .
- Two jobs compatible if they don't overlap.
- Goal: find maximum weight subset of mutually compatible jobs.

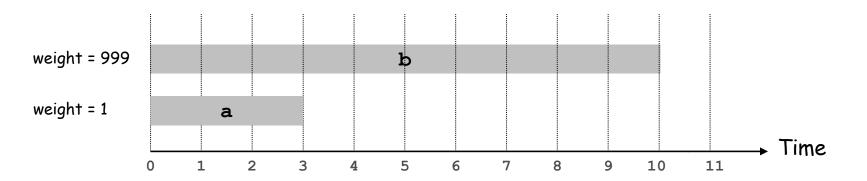


Unweighted Interval Scheduling Review

Recall. Greedy algorithm works if all weights are 1.

- Consider jobs in ascending order of finish time.
- Add job to subset if it is compatible with previously chosen jobs.

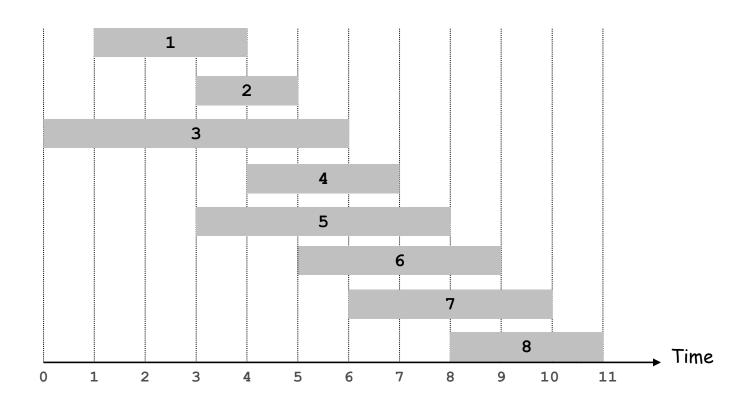
Observation. Greedy algorithm can fail spectacularly if arbitrary weights are allowed.



Weighted Interval Scheduling

Notation. Label jobs by finishing time: $f_1 \le f_2 \le ... \le f_n$. Def. p(j) = largest index i < j such that job i is compatible with j.

Ex: p(8) = 5, p(7) = 3, p(2) = 0.



Dynamic Programming: Binary Choice

Notation. OPT(j) = value of optimal solution to the problem consisting of job requests 1, 2, ..., j.

- Case 1: OPT selects job j.
 - collect profit v_j
 - can't use incompatible jobs { p(j) + 1, p(j) + 2, ..., j 1 }
 - must include optimal solution to problem consisting of remaining compatible jobs 1, 2, ..., p(j)

optimal substructure

- Case 2: OPT does not select job j.
 - must include optimal solution to problem consisting of remaining compatible jobs 1, 2, ..., j-1

$$OPT(j) = \begin{cases} 0 & \text{if } j = 0\\ \max \{ v_j + OPT(p(j)), OPT(j-1) \} & \text{otherwise} \end{cases}$$

Weighted Interval Scheduling: Brute Force

Brute force algorithm.

```
Input: n, s_1,...,s_n, f_1,...,f_n, v_1,...,v_n

Sort jobs by finish times so that f_1 \leq f_2 \leq ... \leq f_n.

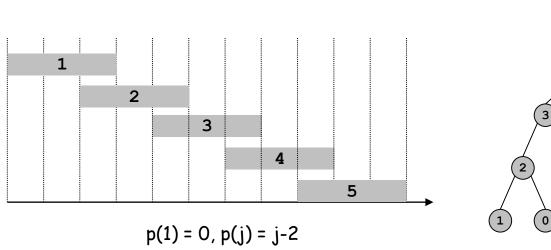
Compute p(1), p(2), ..., p(n)

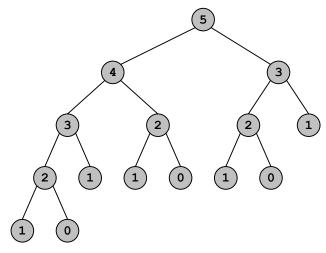
Compute-Opt(j) {
   if (j = 0)
      return 0
   else
      return max(v_j + Compute-Opt(p(j)), Compute-Opt(j-1))
}
```

Weighted Interval Scheduling: Brute Force

Observation. Recursive algorithm fails spectacularly because of redundant sub-problems \Rightarrow exponential algorithms.

Ex. Number of recursive calls for family of "layered" instances grows like Fibonacci sequence.





Weighted Interval Scheduling: Memoization

Memoization. Store results of each sub-problem in a cache; lookup as needed.

```
Input: n, s_1, ..., s_n, f_1, ..., f_n, v_1, ..., v_n
Sort jobs by finish times so that f_1 \le f_2 \le \ldots \le f_n.
Compute p(1), p(2), ..., p(n)
for j = 1 to n
   M[j] = empty global array
M[0] = 0
M-Compute-Opt(j) {
   if (M[j] is empty)
      M[j] = max(v_j + M-Compute-Opt(p(j)), M-Compute-Opt(j-1))
   return M[j]
```

Weighted Interval Scheduling: Running Time

Claim. Memoized version of algorithm takes O(n log n) time.

- Sort by finish time: O(n log n).
- Computing $p(\cdot)$: O(n log n) via sorting by start time.
- M-Compute-Opt(j): each invocation takes O(1) time and either
 - (i) returns an existing value M[j]
 - (ii) fills in one new entry M[j] and makes two recursive calls
- Progress measure Φ = # nonempty entries of M[].
 - initially Φ = 0, throughout $\Phi \leq n$.
 - (ii) increases Φ by $1 \Rightarrow$ at most 2n recursive calls.
- Overall running time of M-Compute-Opt (n) is O(n). •

Remark. O(n) if jobs are pre-sorted by start and finish times.

Weighted Interval Scheduling: Finding a Solution

- Q. Dynamic programming algorithms computes optimal value. What if we want the solution itself?
- A. Do some post-processing.

```
Run M-Compute-Opt(n)
Run Find-Solution(n)

Find-Solution(j) {
   if (j = 0)
      output nothing
   else if (v<sub>j</sub> + M[p(j)] > M[j-1])
      print j
      Find-Solution(p(j))
   else
      Find-Solution(j-1)
}
```

• # of recursive calls \leq n \Rightarrow O(n).

Weighted Interval Scheduling: Bottom-Up

Bottom-up dynamic programming. Unwind recursion.

```
Input: n, s_1,...,s_n, f_1,...,f_n, v_1,...,v_n

Sort jobs by finish times so that f_1 \le f_2 \le ... \le f_n.

Compute p(1), p(2), ..., p(n)

Iterative-Compute-Opt {

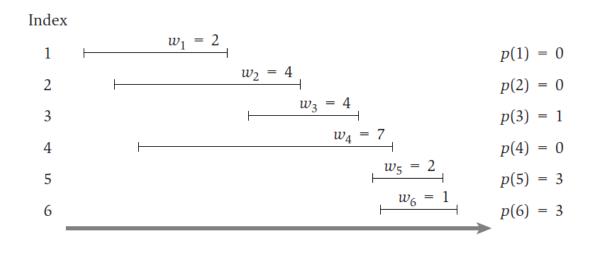
M[0] = 0

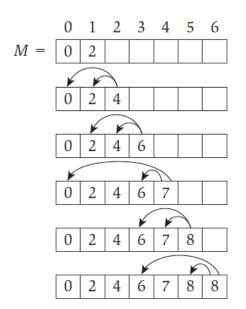
for j = 1 to n

M[j] = max(v_j + M[p(j)], M[j-1])
}
```

previously computed values

An example of Iterative-Compute-Opt





Outline

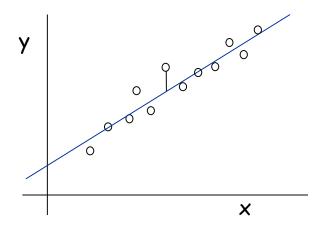
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Segmented Least Squares

Least squares.

- Foundational problem in statistic and numerical analysis.
- Given n points in the plane: $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$.
- Find a line y = ax + b that minimizes the sum of the squared error:

$$SSE = \sum_{i=1}^{n} (y_i - ax_i - b)^2$$



Solution. Calculus \Rightarrow min error is achieved when

$$a = \frac{n \sum_{i} x_{i} y_{i} - (\sum_{i} x_{i}) (\sum_{i} y_{i})}{n \sum_{i} x_{i}^{2} - (\sum_{i} x_{i})^{2}}, \quad b = \frac{\sum_{i} y_{i} - a \sum_{i} x_{i}}{n}$$

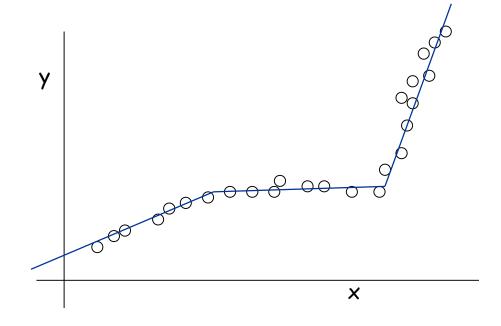
Segmented Least Squares

Segmented least squares.

- Points lie roughly on a sequence of several line segments.
- Given n points in the plane $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with $x_1 < x_2 < \ldots < x_n$, find a sequence of lines that minimizes f(x).

Q. What's a reasonable choice for f(x) to balance accuracy and parsimony?

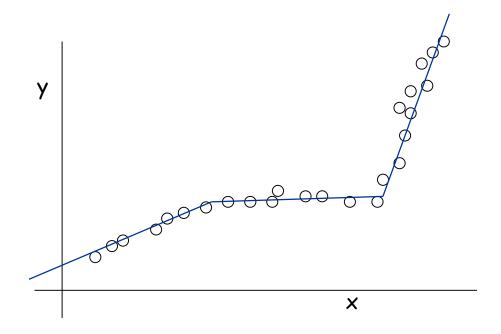
number of lines



Segmented Least Squares

Segmented least squares.

- Points lie roughly on a sequence of several line segments.
- Given n points in the plane $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ with $x_1 < x_2 < \ldots < x_n$, find a sequence of lines that minimizes:
 - the sum of the sums of the squared errors E in each segment
 - the number of lines L
- Tradeoff function: E + c L, for some constant c > 0.



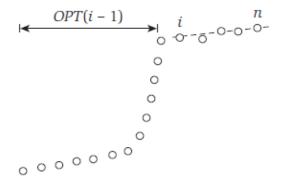
Dynamic Programming: Multiway Choice

Notation.

- OPT(j) = minimum cost for points $p_1, p_{i+1}, \ldots, p_j$.
- e(i, j) = minimum sum of squares for points $p_i, p_{i+1}, \ldots, p_i$

To compute OPT(j):

- Last segment uses points p_i , p_{i+1} , ..., p_j for some i.
- Cost = e(i, j) + c + OPT(i-1).



$$OPT(j) = \begin{cases} 0 & \text{if } j = 0\\ \min_{1 \le i \le j} \left\{ e(i, j) + c + OPT(i - 1) \right\} & \text{otherwise} \end{cases}$$

Segmented Least Squares: Algorithm

```
INPUT: p_1, \dots, p_N c
Segmented-Least-Squares() {
   M[0] = 0
   for j = 1 to n
       for i = 1 to j
           compute the least square error e<sub>ij</sub> for
           the segment p<sub>i</sub>,..., p<sub>i</sub>
   for j = 1 to n
       M[j] = \min_{1 \le i \le j} (e_{ij} + c + M[i-1])
   return M[n]
```

Running time. $O(n^3)$. \checkmark can be improved to $O(n^2)$ by pre-computing various statistics

■ Bottleneck = computing e(i, j) for $O(n^2)$ pairs, O(n) per pair using previous formula.

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Knapsack Problem

Knapsack problem.

- Given n objects and a "knapsack."
- Item i weighs $w_i > 0$ kilograms and has value $v_i > 0$.
- Knapsack has capacity of W kilograms.
- Goal: fill knapsack so as to maximize total value.

Ex: { 3, 4 } has value 40.

W = 11

#	value	weight
1	1	1
2	6	2
3	18	5
4	22	6
5	28	7

Greedy: repeatedly add item with maximum ratio v_i / w_i .

Ex: $\{5, 2, 1\}$ achieves only value = $35 \Rightarrow \text{greedy not optimal}$.

Dynamic Programming: False Start

Def. OPT(i) = max profit subset of items 1, ..., i.

- Case 1: OPT does not select item i.
 - OPT selects best of { 1, 2, ..., i-1 }
- Case 2: OPT selects item i.
 - accepting item i does not immediately imply that we will have to reject other items
 - without knowing what other items were selected before i,
 we don't even know if we have enough room for i

Conclusion. Need more sub-problems!

Dynamic Programming: Adding a New Variable

Def. OPT(i, w) = max profit subset of items 1, ..., i with weight limit w.

- Case 1: OPT does not select item i.
 - OPT selects best of { 1, 2, ..., i-1 } using weight limit w
- Case 2: OPT selects item i.
 - new weight limit = w wi
 - OPT selects best of { 1, 2, ..., i-1 } using this new weight limit

```
\mathit{OPT}(i,\!w) = \begin{cases} 0 & \text{if } i = 0 \\ 0 & \text{if } w = 0 \\ \mathit{OPT}(i-1,\!w) & \text{if } w_i > w \\ \max \left\{ \mathit{OPT}(i-1,\!w), v_i + \mathit{OPT}(i-1,\!w-w_i) \right\} & \text{otherwise} \end{cases}
```

Knapsack Problem: Bottom-Up

Knapsack. Fill up an n-by-W array.

```
Input: n, W, w_1, \dots, w_N, v_1, \dots, v_N
for w = 0 to W
   M[0, w] = 0
for i = 1 to n
   for w = 1 to W
      if (w_i > w)
          M[i, w] = M[i-1, w]
      else
          M[i, w] = \max \{M[i-1, w], v_i + M[i-1, w-w_i]\}
return M[n, W]
```

Knapsack Algorithm

_____ W + 1 _____

		0	1	2	3	4	5	6	7	8	9	10	11
n + 1	ф	0	0	0	0	0	0	0	0	0	0	0	0
	{ 1 }	0	1	1	1	1	1	1	1	1	1	1	1
	{ 1, 2 }	0	1	6	7	7	7	7	7	7	7	7	7
	{1,2,3}	0	1	6	7	7	18	19	24	25	25	25	25
	{1,2,3,4}	0	1	6	7	7	18	22	24	28	29	29	40
	{1,2,3,4,5}	0	1	6	7	7	18	22	28	29	34	34	40

OPT: { 4, 3 }

value = 22 + 18 = 40

W = 11

Item	Value	Weight
1	1	1
2	6	2
3	18	5
4	22	6
5	28	7

Knapsack Problem: Running Time

Running time. $\Theta(n W)$.

- Not polynomial in input size!
- "Pseudo-polynomial."
- Decision version of Knapsack is NP-complete.

Recover an optimal set of items.

Use another tabular to memorize the selected item each time.

$$L(i,w) = \begin{cases} L(i-1,w) & \text{if } w_i > w \\ L(i-1,w) & OPT(i-1,w) > v_i + OPT(i-1,w-w_i) \\ i & OPT(i-1,w) <= v_i + OPT(i-1,w-w_i) \end{cases}$$

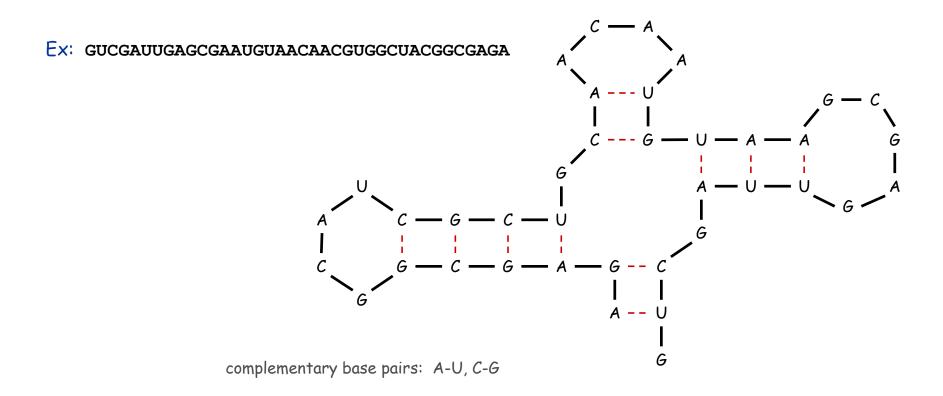
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RNA Secondary Structure

RNA. String B = $b_1b_2...b_n$ over alphabet { A, C, G, U }.

Secondary structure. RNA is single-stranded so it tends to loop back and form base pairs with itself. This structure is essential for understanding behavior of molecule.



RNA Secondary Structure

Secondary structure. A set of pairs $S = \{(b_i, b_j)\}$ that satisfy:

- [Watson-Crick.] S is a matching and each pair in S is a Watson-Crick complement: A-U, U-A, C-G, or G-C.
- [No sharp turns.] The ends of each pair are separated by at least 4 intervening bases. If $(b_i, b_j) \in S$, then i < j 4.
- [Non-crossing.] If (b_i, b_j) and (b_k, b_l) are two pairs in S, then we cannot have i < k < j < l.

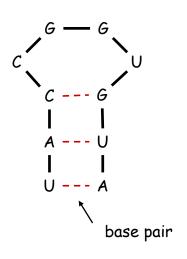
Free energy. Usual hypothesis is that an RNA molecule will form the secondary structure with the optimum total free energy.

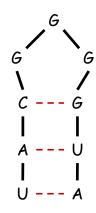
approximate by number of base pairs

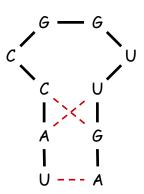
Goal. Given an RNA molecule $B = b_1b_2...b_n$, find a secondary structure S that maximizes the number of base pairs.

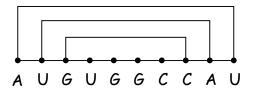
RNA Secondary Structure: Examples

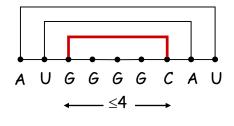
Examples.

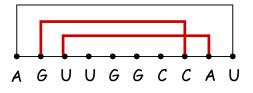












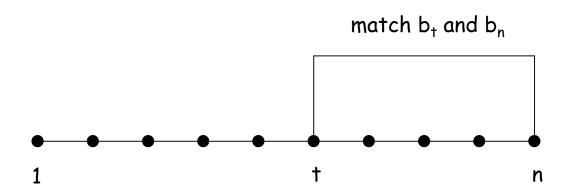
ok

sharp turn

crossing

RNA Secondary Structure: Subproblems

First attempt. OPT(j) = maximum number of base pairs in a secondary structure of the substring $b_1b_2...b_j$.



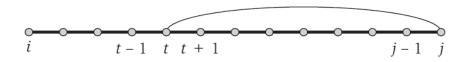
Difficulty. Results in two sub-problems.

- Finding secondary structure in: $b_1b_2...b_{t-1}$. $\leftarrow OPT(t-1)$
- Finding secondary structure in: $b_{t+1}b_{t+2}...b_{n-1}$. ← need more sub-problems

Dynamic Programming Over Intervals

Notation. OPT(i, j) = maximum number of base pairs in a secondary structure of the substring $b_i b_{i+1} ... b_j$.

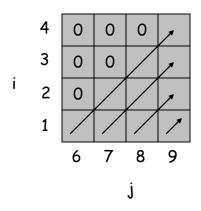
- Case 1. If $i \ge j 4$.
 - OPT(i, j) = 0 by no-sharp turns condition.
- Case 2. Base b_i is not involved in a pair.
 - OPT(i, j) = OPT(i, j-1)
- Case 3. Base b_i pairs with b_t for some $i \le t < j 4$.
 - non-crossing constraint decouples resulting sub-problems
 - $OPT(i, j) = 1 + max_{t} \{ OPT(i, t-1) + OPT(t+1, j-1) \}$



Remark. Same core idea in CKY algorithm to parse context-free grammars.

Bottom Up Dynamic Programming Over Intervals

- Q. What order to solve the sub-problems?
- A. Do shortest intervals first.



Running time. $O(n^3)$.

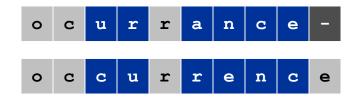
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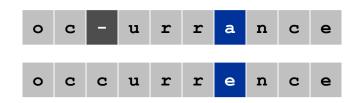
String Similarity

How similar are two strings?

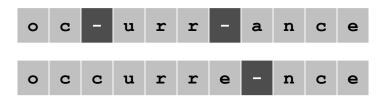
- ocurrance
- occurrence



6 mismatches, 1 gap



1 mismatch, 1 gap



O mismatches, 3 gaps

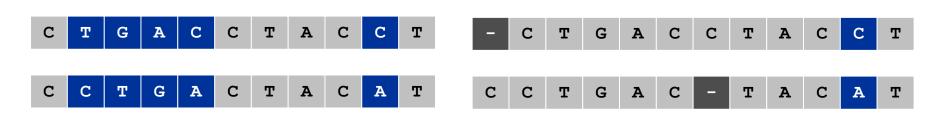
Edit Distance

Applications.

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

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

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



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

$$2\delta$$
 + α_{CA}

Sequence Alignment

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

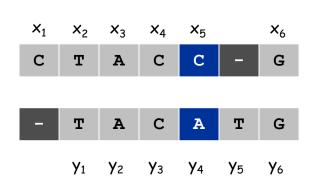
Def. An alignment M is a set of ordered pairs x_i - y_j such that each item occurs in at most one pair and no crossings.

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

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

Ex: CTACCG VS. TACATG.

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



Sequence Alignment: Problem Structure

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

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

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

$$i\delta & \text{if } j = 0$$

Sequence Alignment: Algorithm

```
Sequence-Alignment(m, n, x_1x_2...x_m, y_1y_2...y_n, \delta, \alpha) {
   for i = 0 to m
       M[i, 0] = i\delta
   for j = 0 to n
       M[0, i] = i\delta
   for i = 1 to m
       for j = 1 to n
          M[i, j] = min(\alpha[x_i, y_i] + M[i-1, j-1],
                            \delta + M[i-1, j],
                            \delta + M[i, j-1]
   return M[m, n]
```

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

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

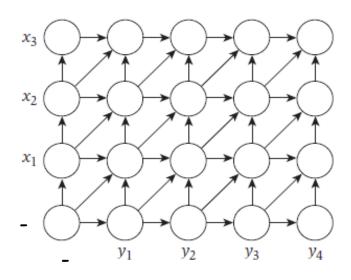
Computational biology: m = n = 100,000. 10 billions ops OK, but 10GB array?

Q. Can we avoid using quadratic space?

A graph-based picture of sequence alignment

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

- Suppose build a two-dimensional m-by-n grid graph Gxy, with the rows labels by symbols in X and the columns labeled by symbols in Y.
- Put costs on edges: the cost of each horizontal and vertical edge is δ , and the cost of the diagonal edge from (i 1, j 1) to (i, j) is α_{x_i, y_i} .



A graph-based picture of sequence alignment

(6.17) Let f(i,j) denote the minimum cost of a path from (0,0) to (i,j) in G_{XY} . Then for all i,j, we have f(i,j) = OPT(i,j).

Proof. We can easily prove this by induction on i + j. When i + j = 0, we have i = j = 0, and indeed f(i, j) = OPT(i, j) = 0.

Now consider arbitrary values of i and j, and suppose the statement is true for all pairs (i', j') with i' + j' < i + j. The last edge on the shortest path to (i, j) is either from (i - 1, j - 1), (i - 1, j), or (i, j - 1). Thus we have

$$\begin{split} f(i,j) &= \min[\alpha_{x_i y_j} + f(i-1,j-1), \delta + f(i-1,j), \delta + f(i,j-1)] \\ &= \min[\alpha_{x_i y_j} + \text{OPT}(i-1,j-1), \delta + \text{OPT}(i-1,j), \delta + \text{OPT}(i,j-1)] \\ &= \text{OPT}(i,j), \end{split}$$

where we pass from the first line to the second using the induction hypothesis, and we pass from the second to the third using (6.16). ■

Outline

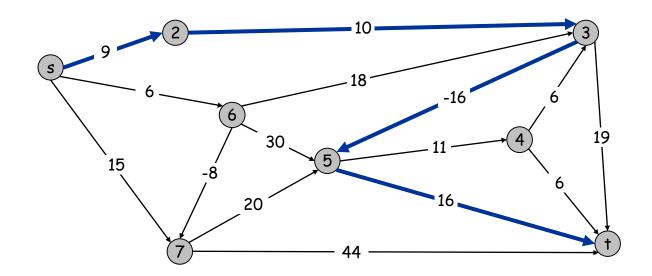
- Overview
- Weighted Interval Scheduling
- Segmented Least Squares
- Knapsack Problem
- · RNA Secondary Structure
- · Sequence Alignment
- · Shortest Paths with negative weights

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.

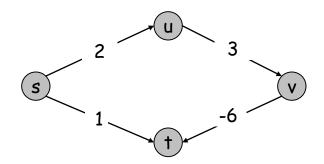
allow negative weights

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.

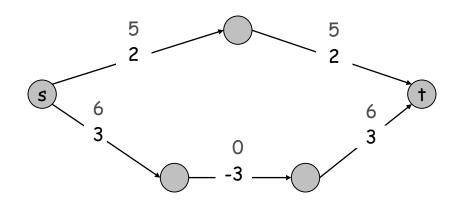


Shortest Paths: Failed Attempts

Dijkstra. Can fail if negative edge costs.

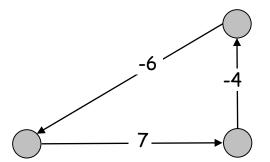


Re-weighting. Adding a constant to every edge weight can fail.

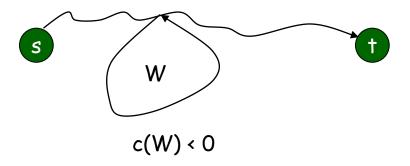


Shortest Paths: Negative Cost Cycles

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

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

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<sub>vw</sub> }
}
```

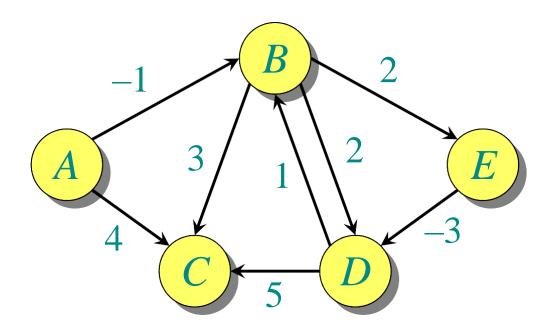
Analysis. $\Theta(mn)$ time, $\Theta(n^2)$ space.

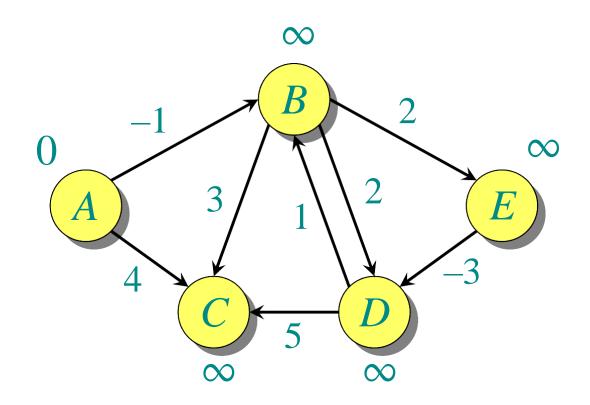
Finding the shortest paths. Maintain a "successor" for each table entry.

Bellman-Ford algorithm

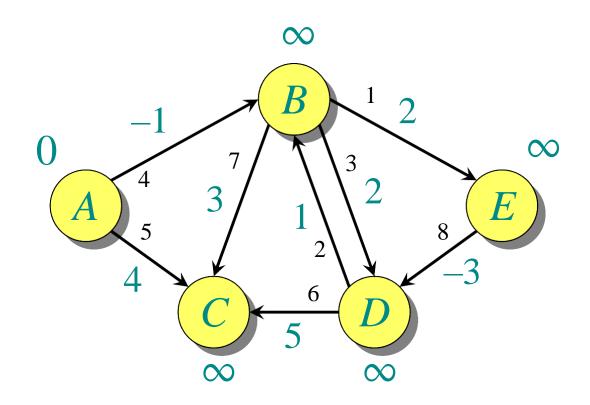
for each
$$v \in V - \{s\}$$
 do $d[v] \leftarrow \infty$ initialization do $d[v] \leftarrow \infty$ for $i \leftarrow 1$ to $|V| - 1$ do for each edge $(u, v) \in E$ do if $d[v] > d[u] + w(u, v)$ relaxation then $d[v] \leftarrow d[u] + w(u, v)$ step for each edge $(u, v) \in E$ do if $d[v] > d[u] + w(u, v)$ then report that a negative-weight cycle exists At the end, $d[v] = \delta(s, v)$, if no negative-weight cycles. Time $= O(VE)$.

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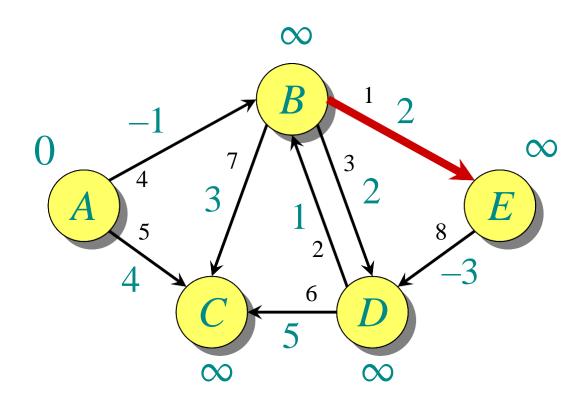


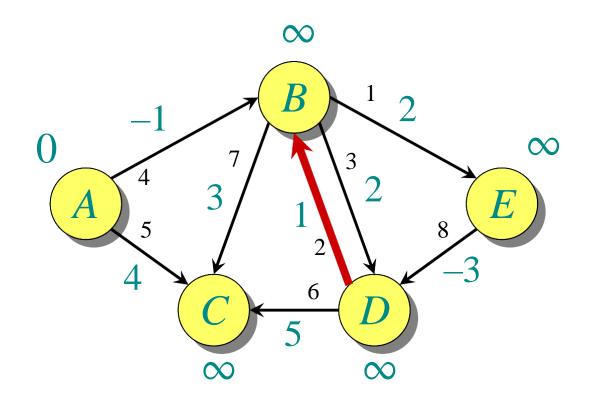


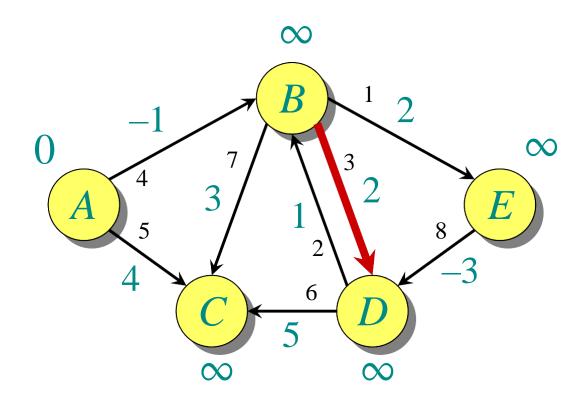
Initialization.

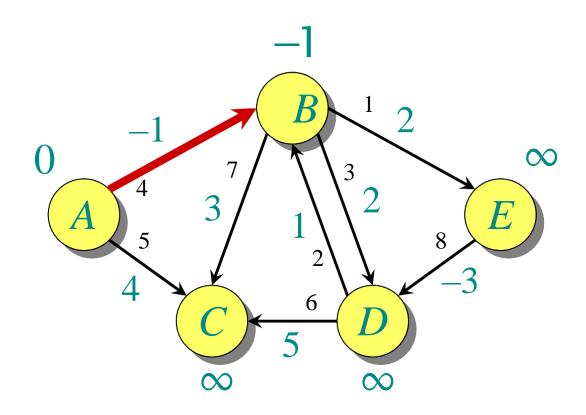


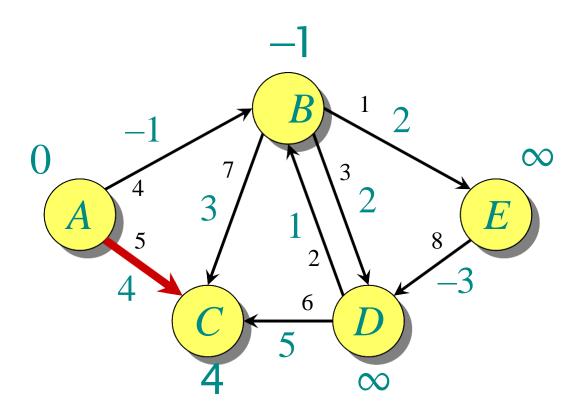
Order of edge relaxation.

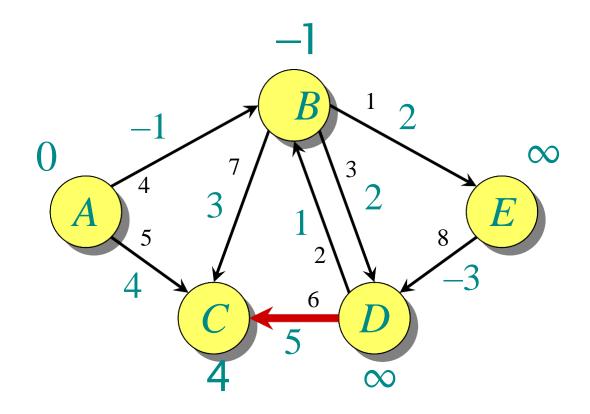


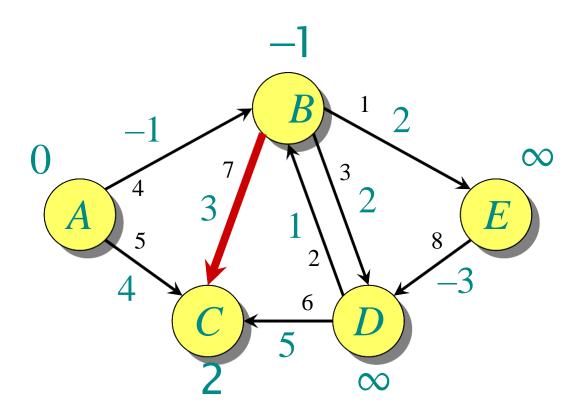


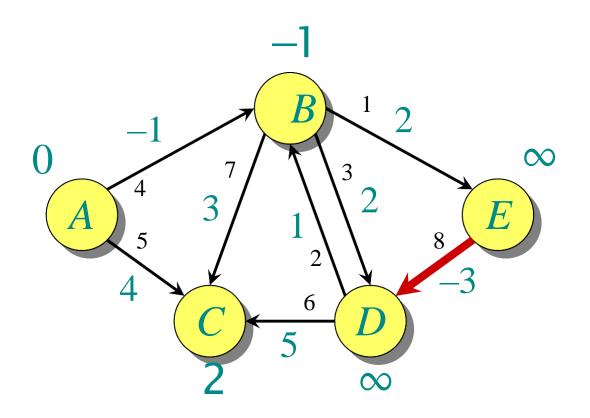


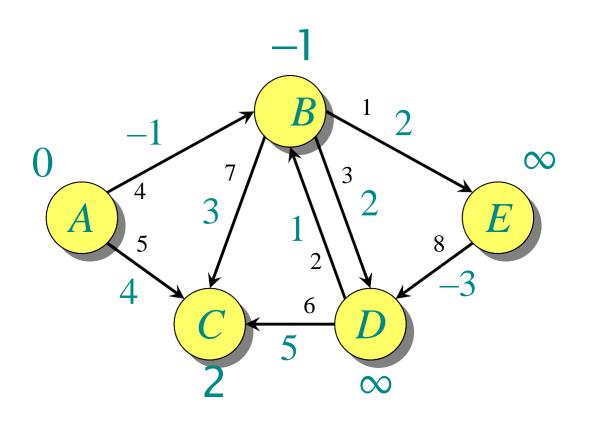




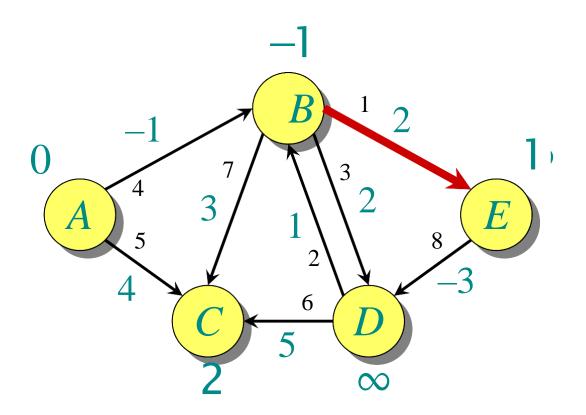


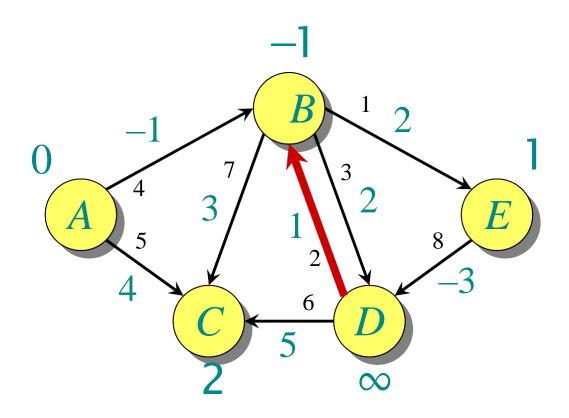


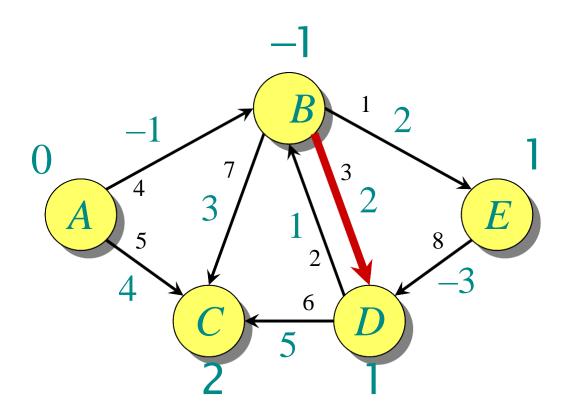


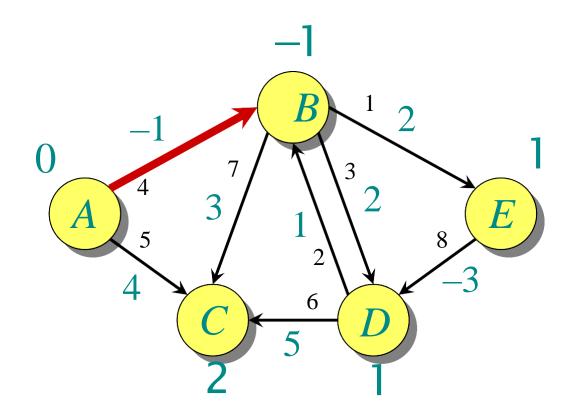


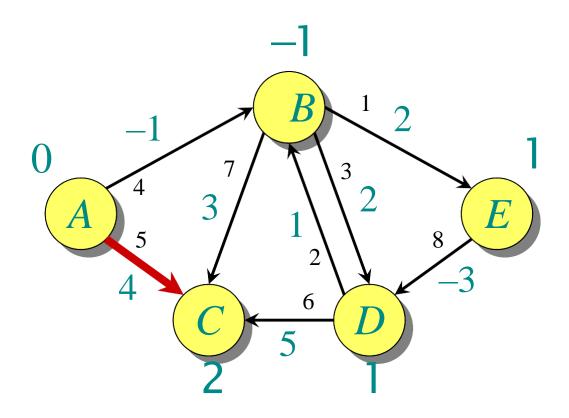
End of pass 1.

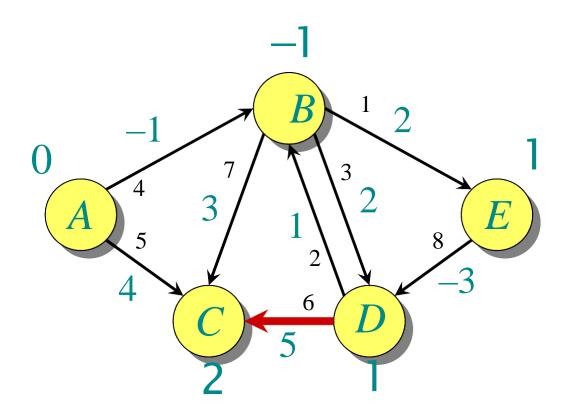


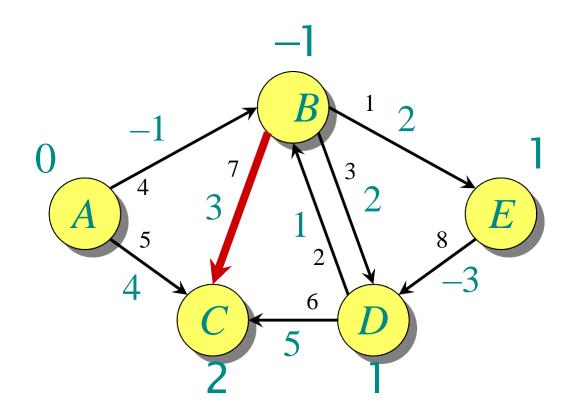


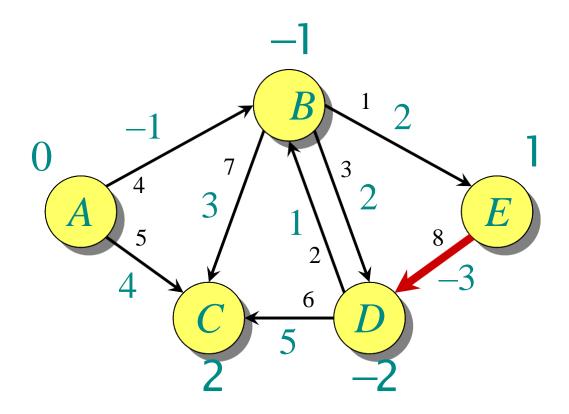


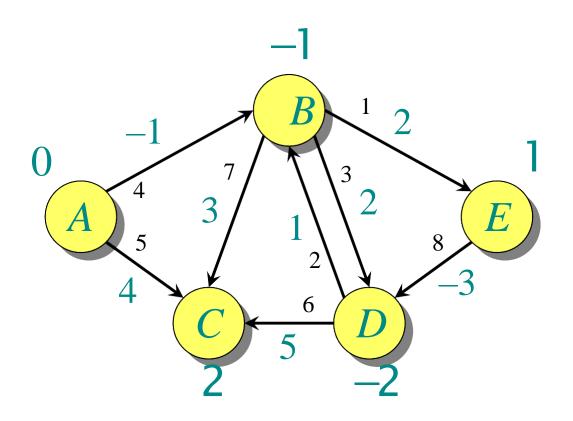












End of pass 2 (and 3 and 4).

Dynamic Programming Summary

Recipe.

- Characterize structure of problem.
- Recursively define value of optimal solution.
- Compute value of optimal solution.
- Construct optimal solution from computed information.

Dynamic programming techniques.

- Binary choice: weighted interval scheduling.
- Multi-way choice: segmented least squares.

Viterbi algorithm for HMM also uses DP to optimize a maximum likelihood tradeoff between parsimony and accuracy

- Adding a new variable: knapsack.
- Dynamic programming over intervals: RNA secondary structure.

CKY parsing algorithm for context-free grammar has similar structure

Top-down vs. bottom-up: different people have different intuitions.