

#### Algorithmic Paradigms

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

Divide-and-conquer. Break up a problem into two 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.

#### Dynamic Programming History

Bellman. Pioneered the systematic study of dynamic programming in the 1950s.

#### Etymology.

- Dynamic programming = planning over time.
- Secretary of Defense was hostile to mathematical research.
- Bellman sought an impressive name to avoid confrontation.
  - "it's impossible to use dynamic in a pejorative sense"
  - "something not even a Congressman could object to"

Reference: Bellman, R. E. Eye of the Hurricane, An Autobiography.

#### Dynamic Programming Applications

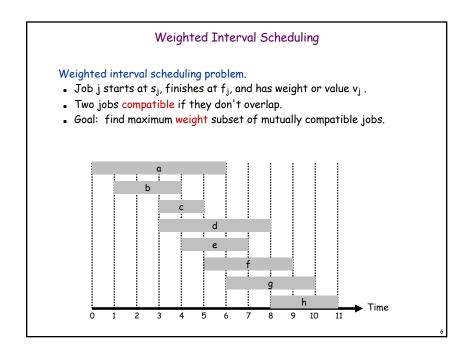
#### Areas.

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

#### Some famous dynamic programming algorithms.

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

6.1 Weighted Interval Scheduling

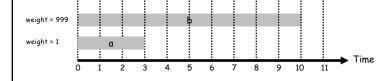


#### Unweighted Interval Scheduling Review

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.

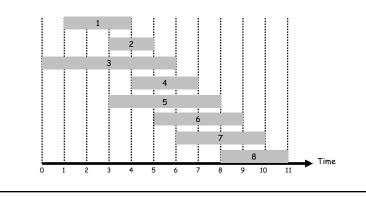
Observation. Greedy algorithm can fail spectacularly if arbitrary weights are allowed.





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.
  - 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

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

```
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 \le f_2 \le ... \le f_n.

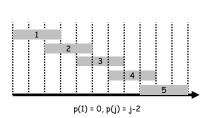
Compute p(1), p(2), ..., p(n)

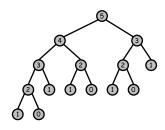
Compute-Opt(j) {
   if (j = 0)
     return 0
   else
     return max(v_j + Compute-Opt(p(j)), Compute-Opt(j-1))
}
```

### Weighted Interval Scheduling: Brute Force

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

 $\ensuremath{\mathsf{Ex}}.$  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<sub>1</sub>,...,s<sub>n</sub>, f<sub>1</sub>,...,f<sub>n</sub>, v<sub>1</sub>,...,v<sub>n</sub>

Sort jobs by finish times so that f<sub>1</sub> ≤ f<sub>2</sub> ≤ ... ≤ f<sub>n</sub>.
Compute p(1), p(2), ..., p(n)

for j = 1 to n
    M[j] = empty ← global array

M[j] = 0

M-Compute-Opt(j) {
    if (M[j] is empty)
        M[j] = max(w<sub>j</sub> + 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) after 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  ${\tt M[j]}$  and makes two recursive calls
- Progress measure  $\Phi$  = # nonempty entries of M[].
  - initially  $\Phi$  = 0, throughout  $\Phi \leq$  n.
  - (ii) increases  $\Phi$  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])
}
```

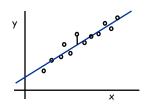
6.3 Segmented Least Squares

#### 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

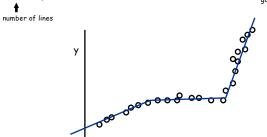
$$a = \frac{n\sum_{i}x_{i}y_{i} - \left(\sum_{i}x_{i}\right)\left(\sum_{i}y_{i}\right)}{n\sum_{i}x_{i}^{2} - \left(\sum_{i}x_{i}\right)^{2}}, \quad b = \frac{\sum_{i}y_{i} - a\sum_{i}x_{i}}{n}$$

#### 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
- $x_1 < x_2 < ... < x_n$ , find a sequence of lines that minimizes f(x).

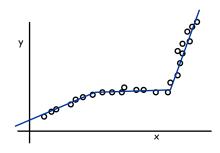
Q. What's a reasonable choice for f(x) to balance accuracy and parsimony?



#### 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
- $x_1 < x_2 < ... < x_n$ , 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<sub>1</sub>, p<sub>i+1</sub>, ..., p<sub>j</sub>.
- e(i, j) = minimum sum of squares for points  $p_i, p_{i+1}, \ldots, p_j$ .

#### 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: n, p<sub>1</sub>,...,p<sub>N</sub>, 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>j</sub>

for j = 1 to n
    M[j] = min<sub>1 ≤ i ≤ j</sub> (e<sub>ij</sub> + c + M[i-1])
    return M[n]
}
```

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

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

# 6.4 Knapsack Problem

#### 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

Item	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  $\Rightarrow$  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

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

```
Knapsack Problem: Bottom-Up
```

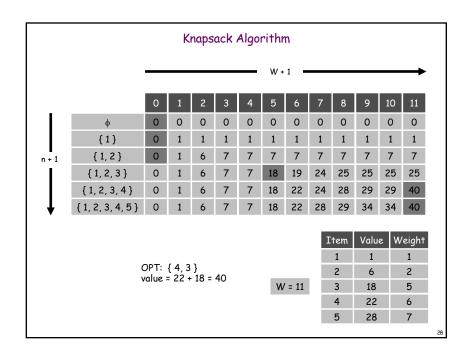
Knapsack. Fill up an n-by-W array.

```
Input: n, w<sub>1</sub>,...,w<sub>N</sub>, v<sub>1</sub>,...,v<sub>N</sub>

for w = 0 to W
   M[0, w] = 0

for i = 1 to n
   for w = 1 to W
        if (w<sub>i</sub> > w)
            M[i, w] = M[i-1, w]
   else
        M[i, w] = max {M[i-1, w], v<sub>i</sub> + M[i-1, w-w<sub>i</sub>]}

return M[n, W]
```



Knapsack Problem: Running Time

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

- Not polynomial in input size!
- "Pseudo-polynomial."
- Decision version of Knapsack is NP-complete. [Chapter 8]

Knapsack approximation algorithm. There exists a polynomial algorithm that produces a feasible solution that has value within 0.01% of optimum. [Section 11.8]

2)

6.5 RNA Secondary Structure

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.

Ex: GUCGAUUGAGCGAAUGUAACAACGUGGCUACGGCGAGA

complementary base pairs: A-U, C-G

#### RNA Secondary Structure

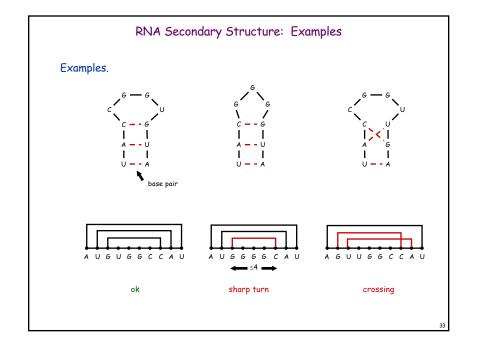
Secondary structure. A set of pairs  $S = \{(b_i, b_j)\}$  that satisfy:

- [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.

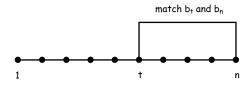
approximate by number of base pairs

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: 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:  $b_1b_2...b_{t-1}$ .
- ← OPT(†-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  $b_ib_{i+1}...b_j$ .

- Case 1. If  $i \ge j 4$ .
- OPT(i, j) = 0 by no-sharp turns condition.
- Case 2. Base b<sub>j</sub> 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
  - $OPT(i, j) = 1 + max_{+} \{ OPT(i, t-1) + OPT(t+1, j-1) \}$

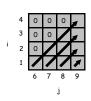
take max over t such that  $i \leq t \lessdot j\text{--}4$  and bt and bj are Watson-Crick complements

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.

```
RNA (b_1, ..., b_n) {
   for k = 5, 6, ..., n-1
      for i = 1, 2, ..., n-k
          j = i + k
          Compute M[i, j]
   return M[1, n]
                       using recurrence
```



Running time. O(n3). Final recurrence

 $OPT(i, j) = max(OPT(I, j-1), 1 + max_{t} \{ OPT(i, t-1) + OPT(t+1, j-1) \})$ 

#### Dynamic Programming Summary

- 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. 

  DP to optimize a maximum likelihood tradeoff between parsimony and accuracy

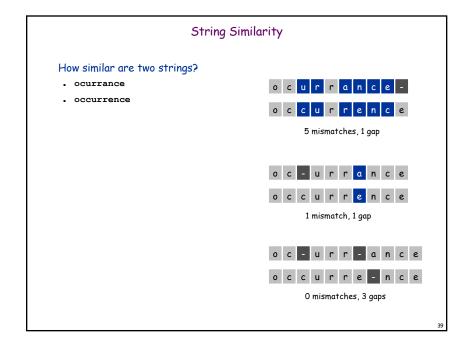
Viterbi algorithm for HMM also uses

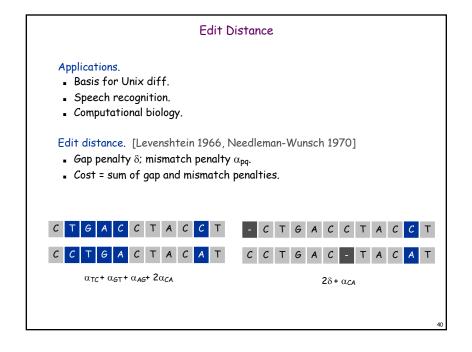
- Adding a new variable: knapsack.
- Dynamic programming over intervals: RNA secondary structure.

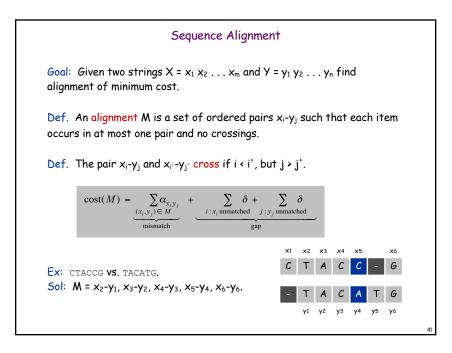
CKY parsing algorithm for context-free

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

6.6 Sequence Alignment







#### Sequence Alignment: Problem Structure

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

- Case 1: OPT matches x<sub>i</sub>-y<sub>j</sub>.
  - 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 xi unmatched.
  - pay gap for  $x_i$  and min cost of aligning  $x_1\,x_2\ldots\,x_{i\text{-}1}$  and  $y_1\,y_2\ldots y_j$
- Case 2b: OPT leaves y, unmatched.
  - pay gap for  $y_j$  and min cost of aligning  $x_1\,x_2\ldots x_i$  and  $y_1\,y_2\ldots y_{j\text{-}1}$

$$OPT(i,j) = \left\{ \begin{array}{ll} j\delta & \text{if } i=0 \\ \\ min \\ \delta + OPT(i-1,j-1) \\ \delta + OPT(i,j-1) \\ \\ i\delta & \text{if } j=0 \end{array} \right.$$

#### Sequence Alignment: Algorithm

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?

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## 6.7 Sequence Alignment in Linear Space

Optional - not required.

Sequence Alignment: Linear Space (optional)

Q. Can we avoid using quadratic space?

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

- Compute OPT(i, ·) from OPT(i-1, ·).
- 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.

