

## 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

## Dynamic Programming Applications

Areas.

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

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"

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

$\square$

## 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

Weighted interval scheduling problem

- 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.


Let's try to understand structure of optimal solution

Case 1: Suppose birdy whispered in your ear that the job with the final finish time was not in the solution

Case 2: Suppose birdy whispered in your ear that the job with the final finish time was in the solution

In each of these cases, what can we say about the optimal solution?

Weighted Interval Scheduling: Brute Force
Observation. Recursive algorithm fails spectacularly $\Rightarrow$ exponential algorithms.

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

$p(1)=0, p(j)=j-2$


## Weighted Interval Scheduling

Notation. Label jobs by finishing time: $f_{1} \leq f_{2} \leq \ldots \leq f_{n}$. Def. $p(j)=$ largest index $i<j$ such that $j o b i$ is compatible with $j$.

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


| j | $\mathrm{P}(\mathrm{i})$ |
| :--- | :--- |
| 0 | - |
| 1 | 0 |
| 2 | 0 |
| 3 | 0 |
| 4 | 1 |
| 5 | 0 |
| 6 | 2 |
| 7 | 3 |
| 8 | 5 | 10

of job requests $1,2, \ldots$,

- Case 1: OPT selects job j
can't use incompatible jobs $\{p(j)+1, p(j)+2, \ldots, j-1\}$
- must include optimal solution to problem consisting of remaining compatible jobs $1,2, \ldots, p(j)$
- 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)={}
{}
if j=0
```

Brute force algorithm.
Weighted Interval Scheduling: Brute Force

```
Input: n, s
Sort jobs by finish times so that f}\mp@subsup{f}{1}{}\leq\mp@subsup{f}{2}{}\leq\ldots\leq\mp@subsup{f}{n}{}
Compute p(1), p(2),\ldots,p(n)
Compute-Opt(j) {
            if ( }j=0
            else
            return max(vj + 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.

$p(1)=0, p(j)=j-2$


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

```
Input: n, s}\mp@subsup{\mathbf{s}}{1}{},\ldots,\mp@subsup{\mathbf{s}}{\textrm{n}}{},\mp@subsup{\mathbf{f}}{1}{},\ldots,\mp@subsup{f}{n}{},\mp@subsup{\mathbf{v}}{1}{},\ldots,\mp@subsup{\mathbf{v}}{\mathbf{n}}{
Sort jobs by finish times so that f}\mp@subsup{f}{1}{}\leq\mp@subsup{f}{2}{}\leq\ldots\leq\mp@subsup{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(w w + M-Compute-Opt(p(j)), M-Compute-Opt(j-1))
        eturn M[j]
}
```


## Weighted Interval Scheduling: Running Time

## Weighted Interval Scheduling: Bottom-Up

Bottom-up dynamic programming. Unwind recursion.
Sort by finish time: $O(n \log n$ )

- Computing $\mathrm{p}(\cdot): O(n)$ 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 $\mathrm{M}[\mathrm{j}]$ 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 $2 n$ 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.

```
Input: n, s
Sort jobs by finish times so that f}\mp@subsup{f}{1}{}\leq\mp@subsup{f}{2}{}\leq\ldots\leq\mp@subsup{f}{n}{
Compute p(1), p(2), .., p(n)
Iterative-Compute-Opt {
    m[0] = 0
        for j = 1 to n
            M[j] = max (vj + M[p(j)],M[j-1])
}
```



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
```



```
        print j
        Find-Solution(p(j))
    else
        Find-Solution(j-1)
}
```

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

## Segmented Least Squares

## Least squares.

- Foundational problem in statistic and numerical analysis.
- Given $n$ points in the plane: $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)$.
- Find $a$ line $y=a x+b$ that minimizes the sum of the squared error

```
SSE = 住 ( (yi-a\mp@subsup{x}{i}{}-b\mp@subsup{)}{}{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 $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)$ 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?
goodness of fit
1



## Segmented Least Squares

Segmented least squares.

- Points lie roughly on a sequence of several line segments.
- Given $n$ points in the plane $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)$ 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 $p_{i}, p_{i+1}, \ldots, p_{j}$

To compute OPT(j)

- Last segment uses points $p_{i}, p_{i+1}, \ldots, p_{j}$ for some $i$.
- Cost $=e(i, j)+c+\operatorname{OPT}(i-1)$.

```
OPT(j)={}
    {\mp@subsup{m}{1\leqslanti\leqj}{}{e(i,j)+c+OPT(i-1)} otherwise
```

Segmented Least Squares: Algorithm

```
INPUT: n, p
Segmented-Least-Squares() {
    M[0] = 0
        j=1 to n
            or i = 1 to j
                compute the least square error ( }\mp@subsup{e}{ij}{}\mathrm{ for
            the segment }\mp@subsup{p}{i}{},\ldots,\mp@subsup{p}{j}{
        for j = 1 to n
            M[j] = min l_isj}(\mp@subsup{e}{ij}{}+c+M[i-1]
        return M[n]
}
```

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

- Bottleneck = computing e $(i, j)$ for $O\left(n^{2}\right)$ 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

| 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 $1, \ldots, i$.

- Case 1: OPT does not select item i.

OPT selects best of $\{1,2, \ldots, i-1\}$

- 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' $\dagger$ even know if we have enough room for i

Conclusion. Need more sub-problems!

Dynamic Programming: Adding a New Variable

Def. $\operatorname{OPT}(i, w)=\max$ profit subset of items $1, \ldots, i$ with weight limit $w$.

- Case 1: OPT does not select item i.

OPT selects best of $\{1,2, \ldots, i-1\}$ using weight limit $w$

- Case 2: OPT selects item i.
- new weight limit $=w-w_{i}$
- OPT selects best of $\{1,2, \ldots, i-1\}$ using this new weight limit
$O P T(i, w)= \begin{cases}0 & \text { if } \mathrm{i}=0 \\ \operatorname{OPT}(i-1, w) & \text { if } \mathrm{w}_{\mathrm{i}}>\mathrm{w} \\ \max \{O P T(i-1, w), & \left.v_{i}+\operatorname{OPT}\left(i-1, w-w_{i}\right)\right\} \\ \text { otherwise }\end{cases}$



## Knapsack Problem: Running Time

Running time. $\Theta(n \mathrm{~W})$.

- 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]
6.5 RNA Secondary Structure

## RNA Secondary Structure

RNA. String $B=b_{1} b_{2} \ldots b_{n}$ 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: gucgauugagcganuguancancgugccuacgccgaca


## RNA Secondary Structure

Secondary structure. A set of pairs $S=\left\{\left(b_{i}, b_{j}\right)\right\}$ that satisfy:

- [Watson-Crick.]
- S is a matching and
each pair in S is a Watson-Crick pair: 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 $\left(b_{i}, b_{j}\right) \in S$, then $i<j-4$.
- [Non-crossing.] If $\left(b_{i}, b_{j}\right)$ and $\left(b_{k}, b_{l}\right)$ are two pairs in $S$, then we cannot have $\mathrm{i}<\mathrm{k}<\mathrm{j}<\mathrm{l}$

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 $B=b_{1} b_{2} \ldots b_{n}$, find a secondary structure $S$ that maximizes the number of base pairs.

Examples.


RNA Secondary Structure: Subproblems

First attempt. OPT(j) = maximum number of base pairs in a secondary structure of the substring $b_{1} b_{2} \ldots b_{j}$.


Difficulty. Results in two sub-problems

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


## Dynamic Programming Over Intervals

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

- Case 1. If $\mathrm{i} \geq \mathrm{j}-4$

OPT $(\mathrm{i}, \mathrm{j})=0$ by no-sharp turns condition.

- Case 2. Base $b_{j}$ is not involved in a pair - OPT( $\mathrm{i}, \mathrm{j})=\operatorname{OPT}(\mathrm{i}, \mathrm{j}-1)$
- Case 3. Base $b_{j}$ pairs with $b_{\dagger}$ for some $i \leq \dagger<j-4$ - non-crossing constraint decouples resulting sub-problems $-\operatorname{OPT}(\mathrm{i}, \mathrm{j})=1+\max _{t}\{\operatorname{OPT}(\mathrm{i}, \mathrm{t}-1)+\operatorname{OPT}(\mathrm{t}+1, \mathrm{j}-1)\}$

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

## 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

- Adding a new variable: knapsack.
- Dynamic programming over intervals: RNA secondary structure.
$\backslash \begin{gathered}\text { CKY arssing ologorithm for cortext-free } \\ \text { gramman has similir structure }\end{gathered}$

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

Bottom Up Dynamic Programming Over Intervals
Q. What order to solve the sub-problems?
A. Do shortest intervals first.

```
RNA (b, (., , b ) {
        , n-1
            or i=1, 2,
            Compute M[i,j
    seturn M[1,n] using recurren
}
```


${ }_{37}$
6.6 Sequence Alignment


## Edit Distance

Applications.

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

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

- Gap penalty $\delta$; mismatch penalty $\alpha_{p q}$.
- Cost = sum of gap and mismatch penalties.
$\alpha_{T C}+\alpha_{G T}+\alpha_{A G}+2 \alpha_{C A}$
$2 \delta+\alpha_{C A}$

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 $x_{i}-y_{j^{\prime}}$ cross if $i<i^{\prime}$, but $\mathrm{j}>\mathrm{j}^{\prime}$.


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 $x_{1} x_{2} \ldots x_{i}$ 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 $y_{1} y_{2} \ldots y_{j-1}$


```
Sequence Alignment: Algorithm
```

```
Sequence-Alignment (m, n, }\mp@subsup{x}{1}{}\mp@subsup{x}{2}{}\ldots\mp@subsup{x}{m}{},\mp@subsup{y}{1}{}\mp@subsup{y}{2}{}\ldots\mp@subsup{y}{n}{\prime},\delta,\alpha)
```

Sequence-Alignment (m, n, }\mp@subsup{x}{1}{}\mp@subsup{x}{2}{}···\mp@subsup{x}{m}{},\mp@subsup{y}{1}{}\mp@subsup{y}{2}{}···\mp@subsup{y}{n}{\prime},\delta,\alpha)
for i=0 to m
for i=0 to m
M[0,i] = id
M[0,i] = id
for j m = 0 to n
for j m = 0 to n
for i = 1 to m
for i = 1 to m
for j = 1 to n
for j = 1 to n
M[i, j] = min (\alpha[[\mp@subsup{x}{i}{},\mp@subsup{y}{j}{\prime}]+M[i-1, j-1],
M[i, j] = min (\alpha[[\mp@subsup{x}{i}{},\mp@subsup{y}{j}{\prime}]+M[i-1, j-1],
\delta +M[i-1, j],
\delta +M[i-1, j],
{\mp@code{\& % M[1-1, j],}
{\mp@code{\& % M[1-1, j],}
return M[m, n]
return M[m, n]
}
Analysis. $\Theta(\mathrm{mn})$ time and space.
English words or sentences: $m, n \leq 10$.
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 $O(m n)$ 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 $O(m n)$ 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: $f(i, j)=\operatorname{OPT}(i, j)$.



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 $D P$. - Align $x_{q}$ and $y_{n / 2}$.

Conquer: recursively compute optimal alignment in each piece.


## Sequence Alignment: Running Time Analysis

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

Pf. (by induction on $n$ )

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

```
T(m,2) \leqc
T(2,n)\leqcn
T(m,n)\leqcmn+T(q,n/2)+T(m-q,n/2)
```

- Base cases: $\mathrm{m}=2$ or $\mathrm{n}=2$.
- Inductive hypothesis: $T(m, n) \leq 2 \mathrm{cmn}$.
$T(m, n) \leq T(q, n / 2)+T(m-q, n / 2)+c m n$
$\leq 2 c q n / 2+2 c(m-q) n / 2+c m n$
$=c q n+c m n-c q n+c m n$
$=2 \mathrm{cmn}$

