## CSE 421: Introduction to Algorithms

# Dynamic Programming 

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## Dynamic Programming

- Dynamic Programming
- Give a solution of a problem using smaller sub-problems where the parameters of all the possible sub-problems are determined in advance
- Useful when the same sub-problems show up again and again in the solution


## A simple case: <br> Computing Fibonacci Numbers

- Recall $F_{n}=F_{n-1}+F_{n-2}$ and $F_{0}=0, F_{1}=1$
- Recursive algorithm:
- Fibo(n)
if $\mathbf{n}=\mathbf{0}$ then return $(\mathbf{0})$
else if $\mathbf{n}=\mathbf{1}$ then return( $\mathbf{1}$ )
else return(Fibo( $\mathbf{n} \mathbf{- 1}$ )+Fibo( $\mathbf{n} \mathbf{- 2}$ ))


## Call tree - start



## Full call tree



## Memoization (Caching)

- Remember all values from previous recursive calls
- Before recursive call, test to see if value has already been computed
- Dynamic Programming
- Convert memoized algorithm from a recursive one to an iterative one


## Fibonacci <br> Dynamic Programming Version

- FiboDP(n): $\mathrm{F}[0] \leftarrow 0$
$\mathrm{F}[1] \leftarrow 1$
for $\mathbf{i}=\mathbf{2}$ to $\mathbf{n}$ do $F[i] \leftarrow F[i-1]+F[i-2]$
endfor return(F[n])


## Fibonacci: Space-Saving Dynamic Programming

- FiboDP(n): $\mathrm{prev} \leftarrow 0$ curr $\leftarrow 1$
for $\mathbf{i}=\mathbf{2}$ to $\mathbf{n}$ do temp $\leftarrow$ curr curr↔curr+prev prev $\leftarrow$ temp
endfor return(curr)


## Dynamic Programming

- Useful when
- same recursive sub-problems occur repeatedly
- Can anticipate the parameters of these recursive calls
- The solution to whole problem can be figured out with knowing the internal details of how the sub-problems are solved
- principle of optimality
"Optimal solutions to the sub-problems suffice for optimal solution to the whole problem"


## Three Steps to Dynamic Programming

- Formulate the answer as a recurrence relation or recursive algorithm
- Show that the number of different values of parameters in the recursive calls is "small"
- e.g., bounded by a low-degree polynomial
- Can use memoization
- Specify an order of evaluation for the recurrence so that you already have the partial results ready when you need them.


## Weighted Interval Scheduling

- Same problem as interval scheduling except that each request i also has an associated value or weight $\mathbf{w}_{\mathrm{i}}$
- $\mathbf{w}_{\mathrm{i}}$ might be
- amount of money we get from renting out the resource for that time period
- amount of time the resource is being used $\mathbf{w}_{\mathrm{i}}=\mathbf{f}_{\mathrm{i}}-\mathbf{s}_{\mathrm{i}}$
- Goal: Find compatible subset S of requests with maximum total weight


## Greedy Algorithms for Weighted Interval Scheduling?

- No criterion seems to work
- Earliest start time $\mathbf{s}_{\mathbf{i}}$
- Doesn't work
- Shortest request time $\mathrm{f}_{\mathrm{i}} \mathrm{s}_{\mathrm{i}}$
- Doesn't work
- Fewest conflicts
- Doesn't work



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- Earliest finish fime $\mathrm{f}_{\mathrm{i}}$
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- Doesn't work
- Fewest conflicts
- Doesn't work
- Earliest finish fime $\mathrm{f}_{\mathrm{i}}$
- Doesn't work
- Largest weight $\mathbf{w}_{\mathrm{i}}$
- Doesn't work



## Towards Dynamic Programming: Step 1 - A Recursive Algorithm

- Suppose that like ordinary interval scheduling we have first sorted the requests by finish time $f_{i}$ so $\mathrm{f}_{1} \leq \mathrm{f}_{2} \leq \ldots \leq \mathrm{f}_{\mathrm{n}}$
- Say request icomes before request $\mathbf{j}$ if $\mathbf{i}<\mathbf{j}$


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- Say request icomes before request jif i<j
- For any request j let p(j) be
- the largest-numbered request before $j$ that is compatible with j
- or $\mathbf{0}$ if no such request exists



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- Suppose that like ordinary interval scheduling we have first sorted the requests by finish time $f_{i}$ so $\mathrm{f}_{1} \leq \mathrm{f}_{2} \leq \ldots . \mathrm{f}_{\mathrm{n}}$
- Say request icomes before request $\mathbf{j}$ if $\mathbf{i}<\mathbf{j}$
- For any request j let p(j) be
- the largest-numbered request before j that is compatible with j
- or 0 if no such request exists
- Therefore $\{1, \ldots, p(\mathrm{j})\}$ is precisely the set of requests before $\mathbf{j}$ that are compatible with $\mathbf{j}$


## Towards Dynamic Programming: Step 1 - A Recursive Algorithm

- Two cases depending on whether an optimal solution $\mathbf{O}$ includes request $\mathbf{n}$
- If it does include request $\mathbf{n}$ then all other requests in O must be contained in $\{1, \ldots, p(n)\}$


## Towards Dynamic Programming: Step 1 - A Recursive Algorithm

- Two cases depending on whether an optimal solution $\mathbf{O}$ includes request $\mathbf{n}$
- If it does include request $\mathbf{n}$ then all other requests in O must be contained in $\{1, \ldots, p(n)\}$
- Not only that!
- Any set of requests in $\{1, \ldots, p(n)\}$ will be compatible with request $n$
- So in this case the optimal solution O must contain an optimal solution for $\{\mathbf{1}, \ldots, \mathrm{p}(\mathrm{n})\}$
- "Principle of Optimality"


## Towards Dynamic Programming: Step 1 - A Recursive Algorithm

- All subproblems involve requests $\{1, . .$, i $\}$ for some i
- For $\mathbf{i}=\mathbf{1}, \ldots$, n let OPT(i) be the weight of the optimal solution to the problem $\{1, \ldots, i\}$
- The two cases give OPT(n)=max[wn+OPT(p(n)),OPT(n-1)]


## Towards Dynamic Programming: Step 1 - A Recursive Algorithm

- All subproblems involve requests $\{1, . .$, i\} for some i
- For $\mathbf{i}=\mathbf{1}, \ldots, \mathbf{n}$ let OPT(i) be the weight of the optimal solution to the problem $\{1, \ldots, i\}$
- The two cases give OPT(n)=max[wn+OPT(p(n)),OPT(n-1)]
- Also
- $\mathrm{n} \in \mathrm{O}$ iff $\mathrm{w}_{\mathrm{n}}+O P T(\mathrm{p}(\mathrm{n}))>$ OPT(n-1)


## Towards Dynamic Programming: Step 1 - A Recursive Algorithm

- Sort requests and compute array $p[i]$ for each $\mathrm{i}=1, \ldots, \mathrm{n}$

ComputeOpt(n)
if $\mathbf{n}=0$ then return( $\mathbf{0}$ )
else
$\mathbf{u} \leftarrow$ ComputeOpt $(\mathbf{p}[\mathbf{n}])$
$\mathbf{v} \leftarrow$ ComputeOpt(n-1)
if $\mathbf{w}_{\mathbf{n}}+\mathbf{u}>\mathbf{v}$ then return $\left(\mathbf{w}_{\mathbf{n}}+\mathbf{u}\right)$
else return(v)
endif

## Towards Dynamic Programming: Step 2 - Small \# of parameters

- ComputeOpt(n) can take exponential time in the worst case
- $2^{n}$ calls if $p(i)=\mathbf{i}-1$ for every $i$


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There are only $\mathbf{n}$ possible parameters to ComputeOpt

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- ComputeOpt(n) can take exponential time in the worst case
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- Store these answers in an array OPT[n] and only recompute when necessary
- Memoization


## Towards Dynamic Programming: Step 2 - Small \# of parameters

- ComputeOpt(n) can take exponential time in the worst case
- $2^{n}$ calls if $p(i)=i-1$ for every $i$
- There are only n possible parameters to ComputeOpt
- Store these answers in an array OPT[n] and only recompute when necessary
- Memoization
- Initialize OPT[i]=0 for $\mathbf{i}=1, \ldots, n$


## Dynamic Programming: Step 2 - Memoization

ComputeOpt(n)
if $\mathbf{n}=0$ then return $(\mathbf{0})$
else
$\mathbf{u} \leftarrow$ MComputeOpt( $\mathbf{p}[\mathbf{n}]$ )
$\mathbf{v} \leftarrow$ MComputeOpt( $\mathbf{n} \mathbf{- 1}$ )
if $\mathbf{w}_{\mathbf{n}}+\mathbf{u}>\mathbf{v}$ then
return $\left(\mathbf{w}_{\mathbf{n}}+\mathbf{u}\right)$
else return(v)
endif

MComputeOpt(n) if OPT[n]=0 then $\mathbf{v} \leftarrow$ ComputeOpt( $\mathbf{n}$ ) OPT $[\mathbf{n}] \leftarrow \mathbf{v}$ return(v) else return(OPT[n]) endif

## Dynamic Programming Step 3: Iterative Solution

- The recursive calls for parameter $\mathbf{n}$ have parameter values ithat are $<\mathbf{n}$

IterativeComputeOpt(n)
array OPT[0..n]
OPT $[0] \leftarrow 0$
for $\mathrm{i}=1$ to n
if $\mathbf{w}_{\mathbf{i}}+$ OPT $[\mathrm{p}[\mathrm{i}]]>$ OPT $[\mathrm{i}-1]$ then
OPT $[i] \leftarrow \mathbf{w}_{\mathbf{i}}+$ OPT[p[i]]
else OPT $[\mathrm{i}] \leftarrow \mathrm{OPT}[\mathrm{i}-1]$
endif
endfor

## Producing the Solution

IterativeComputeOptSolution(n) array OPT[0..n], Used[1..n] OPT $[0] \leftarrow 0$
for $i=1$ to $n$
if $w_{i}+$ OPT $[p[i]]>O P T[i-1]$ then OPT $[\mathrm{i}] \leftarrow \mathrm{w}_{\mathrm{i}}+$ OPT[p[i]] Used $[i] \leftarrow 1$
else
OPT $[i] \leftarrow$ OPT $[i-1]$
Used $[i] \leftarrow 0$
endif
endfor

$\mathbf{i} \leftarrow \mathbf{n}$
$\mathbf{S} \leftarrow \varnothing$
while i> $\mathbf{0}$ do
if Used $[i]=1$ then
$\mathbf{S} \leftarrow \mathbf{S} \cup\{i\}$
$\mathbf{i} \leftarrow \mathbf{p}[\mathbf{i}]$
else
$\mathbf{i} \leftarrow \mathbf{i}-1$
endif
endwhile

## Example

| $\mathrm{s}_{\mathrm{i}}$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 4 | 2 | 6 | 8 | 11 | 15 | 11 | 12 | 18 |
| $\mathrm{f}_{\mathrm{i}}$ | 7 | 9 | 10 | 13 | 14 | 17 | 18 | 19 | 20 |
| $\mathrm{w}_{\mathrm{i}}$ | 3 | 7 | 4 | 5 | 3 | 2 | 7 | 7 | 2 |
| $\mathrm{p}[\mathrm{i}]$ |  |  |  |  |  |  |  |  |  |
| OPT[i] |  |  |  |  |  |  |  |  |  |
| Used[i] |  |  |  |  |  |  |  |  |  |

## Example

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 4 | 2 | 6 | 8 | 11 | 15 | 11 | 12 | 18 |
|  | 7 | 9 | 10 | 13 | 14 | 17 | 18 | 19 | 20 |
| $\mathrm{w}_{\mathrm{i}}$ | 3 | 7 | 4 | 5 | 3 | 2 | 7 | 7 | 2 |
| p[i] | 0 | 0 | 0 | 1 | 3 | 5 | 3 | 3 | 7 |
| OPT[i] |  |  |  |  |  |  |  |  |  |
| Used[i] |  |  |  |  |  |  |  |  |  |

## Example

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 4 | 2 | 6 | 8 | 11 | 15 | 11 | 12 | 18 |
| $f$ | 7 | 9 | 10 | 13 | 14 | 17 | 18 | 19 | 20 |
| $\mathrm{w}_{\mathrm{i}}$ | 3 | 7 | 4 | 5 | 3 | 2 | 7 | 7 | 2 |
| p[i] OPT[i] | 0 | 0 | 0 | 1 | 3 | 5 | 3 | 3 | 7 |
|  | 3 | 7 | 7 | 8 | 10 | 12 | 14 | 14 | 16 |
| Used[[] | 1 | 1 | 0 | , | 1 | 1 | 1 | 0 | 1 |

## Example

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 4 | 2 | 6 | 8 | 11 | 15 | 11 | 12 | 18 |
|  | 7 | 9 | 10 | 13 | 14 | 17 | 18 | 19 | 20 |
| $\mathrm{w}_{\mathrm{i}}$ | 3 | 7 | 4 | 5 | 3 | 2 | 7 | 7 | 2 |
| $p[i]$ | 0 | 0 | 0 | 1 | 3 | 5 | 3 | 3 | 7 |
| OPT[i] | 3 | 7 | 7 | 8 | 10 | 12 | 14 | 14 | 16 |
| Used[[i] | 1 | 1 | 0 | 1 | 1 | 1 | 1 | 0 | 1 |

$$
S=\{9,7,2\}
$$

## Segmented Least Squares

- Least Squares
- Given a set $\mathbf{P}$ of $\mathbf{n}$ points in the plane $\mathbf{p}_{1}=\left(x_{1}, y_{1}\right), \ldots, p_{n}=\left(x_{n}, y_{n}\right)$ with $x_{1}<\ldots<x_{n}$ determine a line $L$ given by $\mathbf{y}=\mathbf{a x}+\mathbf{b}$ that optimizes the total 'squared error'
- $\operatorname{Error}(\mathbf{L}, \mathbf{P})=\Sigma_{i}\left(\mathbf{y}-\mathbf{a x}_{\mathbf{i}} \mathbf{- b}\right)^{2}$
- A classic problem in statistics
- Optimal solution is known (see text)
- Call this line( $\mathbf{P}$ ) and its error error( $\mathbf{P}$ )


## Least Squares



## Segmented Least Squares

- What if data seems to follow a piece-wise linear model?


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- Number of pieces to choose is not obvious


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- If we chose $\mathbf{n} \mathbf{- 1}$ pieces we could fit with $\mathbf{0}$ error
- Not a fair measure of data fit


## Segmented Least Squares

- What if data seems to follow a piece-wise linear model?
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- Add a penalty of C times the number of pieces to the error to get a total penalty


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- What if data seems to follow a piece-wise linear model?
- Number of pieces to choose is not obvious
- If we chose $\mathbf{n} \mathbf{- 1}$ pieces we could fit with $\mathbf{0}$ error
- Not a fair measure of data fit
- Add a penalty of C times the number of pieces to the error to get a total penalty
- How do we compute a solution with the smallest possible total penalty?


## Segmented Least Squares

- Recursive idea
- If we knew the point $p_{j}$ where the last line segment began then we could solve the problem optimally for points $\mathbf{p}_{1}, \ldots, \mathbf{p}_{\mathrm{j}}$ and combine that with the last segment to get a global optimal solution


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- If we knew the point $p_{j}$ where the last line segment began then we could solve the problem optimally for points $\mathbf{p}_{1}, \ldots, \mathbf{p}_{\mathrm{j}}$ and combine that with the last segment to get a global optimal solution
- Let OPT(j) be the optimal penalty for points $\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{j}\right\}$


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- Recursive idea
- If we knew the point $p_{j}$ where the last line segment began then we could solve the problem optimally for points $\mathbf{p}_{1}, \ldots, \mathbf{p}_{\mathrm{j}}$ and combine that with the last segment to get a global optimal solution
- Let OPT(j) be the optimal penalty for points $\left\{\mathbf{p}_{1}, \ldots, \mathbf{p}_{j}\right\}$
- Total penalty for this solution would be

$$
\operatorname{Error}\left(\left\{\mathbf{p}_{\mathbf{j}}, \ldots, \mathbf{p}_{\mathbf{n}}\right\}\right)+\mathbf{C}+\operatorname{OPT}(\mathbf{j}-\mathbf{1})
$$

## Segmented Least Squares



## Segmented Least Squares

- Recursive idea
- We don't know which point is $p_{j}$
- But we do know that $1 \leq j \leq n$
- The optimal choice will simply be the best among these possibilities


## Segmented Least Squares

- Recursive idea
- We don't know which point is $p_{j}$
- But we do know that $1 \leq j \leq n$
- The optimal choice will simply be the best among these possibilities
- Therefore

$$
\begin{gathered}
\operatorname{OPT}(\mathbf{n})=\min _{1 \leq j \leq n}\left\{\operatorname{Error}\left(\left\{\mathbf{p}_{\mathbf{j}}, \ldots, \mathbf{p}_{\mathbf{n}}\right\}\right)+\mathbf{C}+\right. \\
\operatorname{OPT}(\mathbf{j} \mathbf{- 1})\}
\end{gathered}
$$

## Dynamic Programming Solution

SegmentedLeastSquares(n)
array OPT[0..n]
OPT $[0] \leftarrow 0$
for $\mathrm{i}=1$ to n
OPT $[i] \leftarrow \operatorname{Error}\left\{\left(\mathbf{p}_{1}, \ldots, \mathbf{p}_{i}\right)\right\}+\mathbf{C}$
for $\mathbf{j}=\mathbf{2}$ to $\mathrm{i}-1$
$\mathbf{e} \leftarrow \operatorname{Error}\left\{\left(\mathbf{p}_{\mathbf{j}}, \ldots, \mathbf{p}_{\mathbf{i}}\right)\right\}+\mathbf{C}+$ OPT $[\mathbf{j}-1]$
if $\mathbf{e}<\mathbf{O P T}[i]$ then
OPT $[\mathrm{i}] \leftarrow \mathrm{e}$
endif
endfor
endfor
return(OPT[n])

## Dynamic Programming Solution

```
SegmentedLeastSquares(n)
array OPT[0..n]
array Begin[1..n]
OPT[0]\leftarrow0
for i=1 to n
    OPT[i]<Error{(\mp@subsup{p}{1}{},\ldots,\mp@subsup{p}{i}{})}+C
    Begin[i]\leftarrow1
    for j=2 to i-1
        e\leftarrowE\operatorname{Error}{(\mp@subsup{p}{j}{},\ldots,\mp@subsup{p}{i}{})}+C+OPT[j-1]
        if e<OPT[i] then
            OPT[i]}\leftarrow
                Begin[i]}\leftarrow
        endif
    endfor
endfor
return(OPT[n])
```


## Dynamic Programming Solution

```
SegmentedLeastSquares(n)
array OPT[0..n]
array Begin[1..n]
OPT \([0] \leftarrow 0\)
for \(\mathbf{i}=\mathbf{1}\) to \(\mathbf{n}\)
    OPT \([\mathrm{i}] \leftarrow \operatorname{Error}\left\{\left(\mathbf{p}_{1}, \ldots, \mathrm{p}_{\mathrm{i}}\right)\right\}+\mathrm{C}\)
    \(\operatorname{Begin}[i] \leftarrow 1\)
    for \(\mathrm{j}=2\) to \(\mathrm{i}-1\)
        \(\mathbf{e} \leftarrow \operatorname{Error}\left\{\left(\mathbf{p}_{\mathrm{j}}, \ldots, \mathbf{p}_{\mathrm{i}}\right)\right\}+\mathrm{C}+\mathrm{OPT}[\mathrm{j}-1]\)
        if \(\mathbf{e}<\mathbf{O P T}[\mathbf{i}]\) then
            OPT[i] \(\leftarrow \mathbf{e}\)
            Begin \([\mathrm{i}] \leftarrow \mathrm{j}\)
        endif
    endfor
endfor
return(OPT[n])
```

FindSegments
$\mathbf{i} \leftarrow \mathbf{n}$
$S \leftarrow \varnothing$
while i> 1 do
compute Line $\left(\left\{\mathbf{p}_{\text {Begin }[i]}, \ldots, p_{i}\right\}\right)$
output ( $\mathbf{p}_{\text {Begin }[i]}, \mathbf{p}_{\mathbf{i}}$ ), Line $i \leftarrow$ Begin $[i]$
endwhile

## Knapsack (Subset-Sum) Problem

- Given:
- integer W (knapsack size)
- $\mathbf{n}$ object sizes $\mathbf{x}_{1}, \mathbf{x}_{2}, \ldots, \mathbf{x}_{\mathrm{n}}$
- Find:
- Subset $S$ of $\{\mathbf{1}, \ldots, \mathbf{n}\}$ such that $\sum_{i \in \mathrm{~S}} \mathrm{x}_{\mathrm{i}} \leq \mathbf{W}$ but $\sum_{i \in S} \mathrm{x}_{\mathrm{i}}$ is as large as possible


## Recursive Algorithm

- Let $\mathbf{K}(\mathbf{n}, \mathbf{W})$ denote the problem to solve for $W$ and $x_{1}, x_{2}, \ldots, x_{n}$
- For $\mathrm{n}>0$,
- The optimal solution for $\mathbf{K}(\mathbf{n}, \mathbf{W})$ is the better of the optimal solution for either

$$
K(n-1, W) \text { or } x_{n}+K\left(n-1, W-x_{n}\right)
$$

## Recursive Algorithm

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$$
K(n-1, W) \text { or } x_{n}+K\left(n-1, W-x_{n}\right)
$$

- For $\mathrm{n}=0$
- K(0,W) has a trivial solution of an empty set S with weight 0


## Recursive calls

- Recursive calls on list ...,3, 4, 7



## Common Sub-problems

- Only sub-problems are K(i,w) for
- $\mathbf{i}=0,1, \ldots, n$
- $w=0,1, \ldots, W$
- Dynamic programming solution
- Table entry for each K(i,w)
- OPT - value of optimal soln for first i objects and weight w
- belong flag - is $\mathbf{x}_{\mathbf{i}}$ a part of this solution?


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- Table entry for each K(i,w)
- OPT - value of optimal soln for first i objects and weight w
- belong flag - is $\mathbf{x}_{i}$ a part of this solution?
- Initialize OPT[0,w] for w=0,...,W
- Compute all OPT[i,*] from OPT[i-1,*] for i>0


## Dynamic Knapsack Algorithm

for $\mathbf{w}=\mathbf{0}$ to $\mathbf{W}$; $\mathbf{O P T}[\mathbf{0}, \mathbf{w}] \leftarrow \mathbf{0}$; end for
for $\mathbf{i}=\mathbf{1}$ to $\mathbf{n}$ do
for $\mathbf{w}=\mathbf{0}$ to $\mathbf{W}$ do OPT $[i, w] \leftarrow$ OPT $[i-1, w]$ belong $[i, w] \leftarrow 0$
if $\mathbf{w} \geq \mathbf{x}_{\mathbf{i}}$ then
$\mathrm{val} \leftarrow \mathrm{x}_{\mathrm{i}}+$ OPT $\left[\mathrm{i}-1, \mathrm{w}-\mathrm{x}_{\mathrm{i}}\right]$
if val>OPT[i,w] then OPT $[i, w] \leftarrow$ val belong $[i, w] \leftarrow 1$
end for
end for
return(OPT[n,W])

## Sample execution on 2, 3, 4, 7 with W=15

## Saving Space

- To compute the value OPT of the solution only need to keep the last two rows of OPT at each step
- What about determining the set $S$ ?
- Follow the belong flags $\mathbf{O}(n)$ time
- What about space?


## Three Steps to Dynamic Programming

- Formulate the answer as a recurrence relation or recursive algorithm
- Show that the number of different values of parameters in the recursive algorithm is "small"
- e.g., bounded by a low-degree polynomial
- Specify an order of evaluation for the recurrence so that you already have the partial results ready when you need them.


## RNA Secondary Structure: Dynamic Programming on Intervals

- RNA: sequence of bases
- String over alphabet $\{\mathbf{A}, \mathbf{C}, \mathbf{G}, \mathbf{U}\}$ U-G-U-A-C-C-G-G-U-A-G-U-A-C-A
- RNA folds and sticks to itself like a zipper
- A bonds to U
- C bonds to G
- Bends can't be sharp
- No twisting or criss-crossing
- How the bonds line up is called the RNA secondary structure


## RNA Secondary Structure



ACGAUACUGCAAUCUCUGUGACGAACCCAGCGAGGUGUA

## Another view of

RNA Secondary Structure


## RNA Secondary Structure

- Input: String $\mathbf{x}_{1} \ldots \mathbf{x}_{\mathrm{n}} \in\{\mathbf{A}, \mathbf{C}, \mathbf{G}, \mathbf{U}\}^{*}$
- Output: Maximum size set S of pairs (i,j) such that
- $\left\{\mathbf{x}_{i}, \mathbf{x}_{\mathrm{i}}\right]=\{\mathbf{A}, \mathbf{U}\}$ or $\left\{\mathbf{x}_{\mathrm{i}}, \mathrm{x}_{\mathrm{i}}\right\}=\{\mathbf{C}, \mathbf{G}\}$
- The pairs in S form a matching
- i<j-4 (no sharp bends)
- No crossing pairs
- If $(\mathbf{i}, \mathrm{j})$ and ( $\mathbf{k}, \mathrm{I})$ are in S then it is not the case that they cross as in $\mathrm{i}<\mathbf{k}<\mathrm{j}<1$


## Recursion Solution

- Try all possible matches for the last bas

$\operatorname{OPT}(1 . . \mathrm{j})=\operatorname{MAX}\left(\operatorname{OPT}(1 . . \mathrm{j}-1), 1+\mathrm{MAX}_{\mathrm{k}=1 . . \mathrm{j}-5}(\mathrm{OPT}(1 . . \mathrm{k}-1)+\mathrm{OPT}(\mathrm{k}+1 . . \mathrm{j}-1))\right.$

$$
\mathbf{x}_{\mathrm{k}} \text { matches } \mathrm{x}_{\mathrm{j}}
$$

## Recursion Solution

- Try all possible matches for the last base


OPT(1..j)=MAX(OPT(1..j-1), $1+$ MAX $_{k=1 . . j-5}($ OPT(1..k-1)+OPT(k+1..j-1)) $\mathbf{x}_{\mathrm{k}}$ matches $\mathrm{X}_{\mathrm{j}}$

## Recursion Solution

- Try all possible matches for the last base


OPT(1..k-1) OPT(k+1..j-1)
OPT(1..j)=MAX(OPT(1..j-1),1+MAX ${ }_{k=1 . . j-5}($ OPT(1..k-1)+OPT(k+1..j-1)) $\mathbf{x}_{\mathrm{k}}$ matches $\mathrm{X}_{\mathrm{j}}$

## Recursion Solution

- Try all possible matches for the last base


OPT(1..k-1) OPT(k+1..j-1)
OPT(1..j) $=\operatorname{MAX}\left(\right.$ OPT $(1 . . j-1), 1+$ MAX $_{k=1 . . j-5}(O P T(1 . . k-1)+O P T(k+1 . . j-1))$ $\mathrm{x}_{\mathrm{k}}$ matches $\mathrm{x}_{\mathrm{j}} \quad$ Doesn't start at 1

## Recursion Solution

- Try all possible matches for the last base


OPT(1..k-1)
OPT(k+1..j-1)
OPT(1..j) $=\operatorname{MAX}\left(\right.$ OPT $(1 . . j-1), 1+$ MAX $_{k=1 . . . j-5}(O P T(1 . . k-1)+O P T(k+1 . . j-1))$
General form:

$$
\mathrm{x}_{\mathrm{k}} \text { matches } \mathrm{x}_{\mathrm{j}} \quad \text { Doesn't start at } 1
$$

OPT(i..j)=MAX(OPT(i..j-1),

$$
\begin{aligned}
& \left.1+\text { MAX }_{k=i_{. . j}-5}\left(O P T\left(i_{. .} k-1\right)+O P T(k+1 . . j-1)\right)\right) \\
& \quad \text { x }_{k} \text { matches } x_{j}
\end{aligned}
$$

## RNA Secondary Structure

- 2D Array OPT(i,j) for isj represents optimal \# of matches entirely for segment i..j
- For $\mathrm{j}-\mathrm{i} \leq 4$ set OPT(i, j$)=\mathbf{0}$ (no sharp bends)
- Then compute OPT(i, j) values when $\mathrm{j}-\mathrm{i}=5,6, \ldots, \mathrm{n}-1$ in turn using recurrence.
- Return OPT(1,n)
- Total of $\mathbf{O}\left(\mathrm{n}^{3}\right)$ time
- Can also record matches along the way to produce S
- Similar polynomial-time algorithm for other problems
- Context-Free Language recognition
- Optimal matrix products, etc.
- All use dynamic programming over intervals


## Sequence Alignment: Edit Distance

- Given:
- Two strings of characters $A=a_{1} a_{2} \ldots a_{n}$ and $B=b_{1} b_{2} \ldots b_{m}$
- Find:
- The minimum number of edit steps needed to transform A into B where an edit can be:
- insert a single character
- delete a single character
- substitute one character by another


## Applications

- "diff" utility - where do two files differ
- Version control \& patch distribution save/send only changes
- Molecular biology
- Similar sequences often have similar origin and function
- Similarity often recognizable despite millions or billions of years of evolutionary divergence

```
C A - C G T G A T
```


## Sequence Alignment vs Edit Distance

- Sequence Alignment
- Insert corresponds to aligning with a "-" in the first string
- Cost $\delta$ (in our case 1)
- Delete corresponds to aligning with a "-" in the second string
- Cost $\delta$ (in our case 1)
- Replacement of an a by a b corresponds to a mismatch
- Cost $\alpha_{a b}$ (in our case 1 if $\mathbf{a} \neq \mathbf{b}$ and 0 if $\mathbf{a}=\mathbf{b}$ )
- In Computational Biology this alignment algorithm is attributed to Smith \& Waterman


## GenBank and WGS Statistics



## Recursive Solution

- Sub-problems: Edit distance problems for all prefixes of $A$ and $B$ that don't include all of both $A$ and $B$
- Let $\mathrm{D}(\mathrm{i}, \mathrm{j})$ be the number of edits required to transform $a_{1} a_{2} \ldots a_{i}$ into $b_{1} b_{2} \ldots b_{j}$
- Clearly $\mathrm{D}(0,0)=0$


## Computing D(n,m)

- Imagine how best sequence handles the last characters $\mathrm{a}_{\mathrm{n}}$ and $\mathrm{b}_{\mathrm{m}}$
- If best sequence of operations
- deletes $\mathbf{a}_{\mathrm{n}}$ then $\mathrm{D}(\mathrm{n}, \mathrm{m})=\mathrm{D}(\mathrm{n}-\mathbf{1}, \mathrm{m})+\mathbf{1}$
- inserts $b_{m}$ then $D(n, m)=D(n, m-1)+1$
- replaces $\mathrm{a}_{\mathrm{n}}$ by $\mathrm{b}_{\mathrm{m}}$ then

$$
D(n, m)=D(n-1, m-1)+1
$$

- matches $\mathbf{a}_{\mathbf{n}}$ and $\mathbf{b}_{\mathrm{m}}$ then

$$
D(n, m)=D(n-1, m-1)
$$

## Recursive algorithm $\mathrm{D}(\mathrm{n}, \mathrm{m})$

if $\mathbf{n}=\mathbf{0}$ then return ( $\mathbf{m}$ )
elseif $\mathbf{m}=\mathbf{0}$ then
return( $\mathbf{n}$ )
else
if $a_{n}=b_{m}$ then

endif
return $(\boldsymbol{m i n}\{\mathbf{D}(\mathbf{n}-\mathbf{1}, \mathbf{m})+\mathbf{1}$,
$D(n, m-1)+1$,
D(n-1, m-1) + replace-cost $\}$ )

## Dynamic Programming


endfor
endfor

Example run with AGACATTG and GAGTTA


Example run with AGACATTG and GAGTTA


Example run with AGACATTG and GAGTTA

|  |  | A | G | A | C |  | T |  | G |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Q | 1 | 1 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| $\bigcirc$ | 2 | 1 | 2 | 1 |  |  |  |  |  |
| Q | 3 |  |  |  |  |  |  |  |  |
| $\rightarrow$ | 4 |  |  |  |  |  |  |  |  |
| $\bigcirc$ | 5 |  |  |  |  |  |  |  |  |
| $>$ | 6 |  |  |  |  |  |  |  |  |

Example run with AGACATTG and GAGTTA

|  |  | A | G | A | C | A | T |  | G |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
| Q | 1 | 1 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| $\bigcirc$ | 2 | 1 | 2 | 1 | 2 | 3 | 4 | 5 | 6 |
| Q | 3 | 2 | 1 | 2 | 2 | 3 | 4 | 5 | 5 |
| $\rightarrow$ | 4 |  |  |  |  |  |  |  |  |
| - | 5 |  |  |  |  |  |  |  |  |
| $\bigcirc$ | 6 |  |  |  |  |  |  |  |  |

Example run with AGACATTG and GAGTTA


Example run with AGACATTG and GAGTTA

|  | $\begin{array}{llllllllll}\text { A } & \mathbf{G} & \mathbf{A} & \mathbf{C} & \mathbf{A} & \mathbf{T} & \mathbf{T} & \mathbf{G}\end{array}$ |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $0 \leqslant 1 \leqslant 2 \leqslant 3 \leqslant 4 \leqslant 5 \leqslant 6 \leqslant 7 \leqslant 8$ |  |  |  |  |  |  |  |  |
|  | 1 | 1 | 1 | 2 | 3 | 4 | 5 | 0 | 7 |
| 1 | 2 |  | 2 | 1 | - 2 | 3 | \& 4 | 5 | 6 |
| Q | 3 | 2 | 1 | 2 | 2 | 3 | \& 4 | 5 | 5 |
|  | 4 | 3 | 2 | 2 | 3 | 3 | 3 | 4 | 5 |
|  | 5 | 4 | 3 | 3 | 3 | 4 | 3 | 3 | 4 |
| > | 6 | 5 | 4 | 3 | 4 |  | \& 4 | 4 | 4 |

Example run with AGACATTG and GAGTTA


## Reading off the operations

- Follow the sequence and use each color of arrow to tell you what operation was performed.
- From the operations can derive an optimal alignment

AGACATTG
_ GAG_TTA

## Saving Space

- To compute the distance values we only need the last two rows (or columns)
- O(min(m,n)) space
- To compute the alignment/sequence of operations
- seem to need to store all O(mn) pointers/arrow colors
- Nifty divide and conquer variant that allows one to do this in $\mathbf{O}(\min (\mathbf{m}, \mathbf{n}))$ space and retain $\mathbf{O}(\mathbf{m n})$ time
- In practice the algorithm is usually run on smaller chunks of a large string, e.g. m and n are lengths of genes so a few thousand characters
- Researchers want all alignments that are close to optimal
- Basic algorithm is run since the whole table of pointers ( 2 bits each) will fit in RAM
- Ideas are neat, though


## Saving space

- Alignment corresponds to a path through the table from lower right to upper left
- Must pass through the middle column
- Recursively compute the entries for the middle column from the left
- If we knew the cost of completing each then we could figure out where the path crossed
- Problem
- There are n possible strings to start from.
- Solution
- Recursively calculate the right half costs for each entry in this column using alignments starting at the other ends of the two input strings!
- Can reuse the storage on the left when solving the right hand problem


## Shortest paths with negative cost edges (Bellman-Ford)

- Dijsktra's algorithm failed with negative-cost edges
- What can we do in this case?
- Negative-cost cycles could result in shortest paths with length $-\infty$
- Suppose no negative-cost cycles in G
- Shortest path from s to $\mathbf{t}$ has at most n -1 edges
- If not, there would be a repeated vertex which would create a cycle that could be removed since cycle can't have -ve cost


## Shortest paths with negative cost edges (Bellman-Ford)

- We want to grow paths from s to t based on the \# of edges in the path
- Let Cost(s,t,i)=cost of minimum-length path from s to $t$ using up to i hops.
- $\operatorname{Cost}(\mathbf{v}, \mathbf{t}, \mathbf{0})=\left\{\begin{array}{l}\mathbf{0} \text { if } \mathbf{v}=\mathbf{t} \\ \infty \text { otherwise }\end{array}\right.$
- $\operatorname{Cost}(\mathbf{v}, \mathbf{t}, \mathbf{i})=\min \{\operatorname{Cost}(\mathbf{v}, \mathbf{t}, \mathbf{i}-\mathbf{1})$,

$$
\left.\min _{(\mathrm{v}, \mathbf{w}) \in \mathrm{E}}\left(\mathbf{c}_{\mathrm{vw}}+\operatorname{Cost}(\mathbf{w}, \mathbf{t}, \mathbf{i}-\mathbf{1})\right)\right\}
$$

## Bellman-Ford

- Observe that the recursion for Cost(s,t,i) doesn't change t
- Only store an entry for each vand $i$
- Termed OPT(v,i) in the text
- Also observe that to compute OPT(*, i) we only need OPT(*, $\mathrm{i}-1$ )
- Can store a current and previous copy in O(n) space.


## Bellman-Ford

ShortestPath(G,s,t)
for all $\mathbf{v} \in \mathbf{V}$
OPT[v] $\leftarrow \infty$
OPT $[t] \leftarrow 0$
for $\mathbf{i}=\mathbf{1}$ to $\mathbf{n} \mathbf{- 1}$ do
for all $\mathbf{v} \in \mathbf{V}$ do
O(mn) time
OPT $^{\top}[\mathbf{v}] \leftarrow \min _{(v, w) \in \mathrm{E}}\left(\mathbf{c}_{\mathrm{vw}}+\mathrm{OPT}[\mathbf{w}]\right)$
for all $\mathbf{v} \in \mathbf{V}$ do
OPT $[\mathbf{v}] \leftarrow \min (O P T ’[v], O P T[v])$
return OPT[s]

## Negative cycles

- Claim: There is a negative-cost cycle that can reach $t$ iff for some vertex $\mathbf{v} \in \mathbf{V}$, $\operatorname{Cost}(\mathbf{v}, \mathbf{t}, \mathbf{n})<\operatorname{Cost}(\mathbf{v}, \mathbf{t}, \mathbf{n}-\mathbf{1})$
- Proof:
- We already know that if there aren't any then we only need paths of length up to $\mathrm{n}-1$
- For the other direction
- The recurrence computes Cost(v,t,i) correctly for any number of hops $\mathbf{i}$
- The recurrence reaches a fixed point if for every $\mathbf{v} \in \mathbf{V}$, $\operatorname{Cost}(\mathrm{v}, \mathrm{t}, \mathrm{i})=\operatorname{Cost}(\mathrm{v}, \mathrm{t}, \mathrm{i}-1)$
- A negative-cost cycle means that eventually some $\operatorname{Cost}(\mathbf{v}, \mathrm{t}, \mathrm{i})$ gets smaller than any given bound
- Can't have a -ve cost cycle if for every $\mathbf{v} \in \mathbf{V}$, $\operatorname{Cost}(\mathbf{v}, \mathrm{t}, \mathrm{n})=\operatorname{Cost}(\mathrm{v}, \mathrm{t}, \mathrm{n}-1)$


## Last details

- Can run algorithm and stop early if the OPT and OPT' arrays are ever equal
- Even better, one can update only neighbors v of vertices w with OPT'[w] $\quad$ OPT[w]
- Can store a successor pointer when we compute OPT
- Homework assignment
- By running for step $\mathbf{n}$ we can find some vertex v on a negative cycle and use the successor pointers to find the cycle


## Bellman-Ford



## Bellman-Ford



## Bellman-Ford



## Bellman-Ford



## Bellman-Ford



## Bellman-Ford



## Bellman-Ford



## Bellman-Ford with a DAG

Edges only go from lower to higher-numbered vertices

- Update distances in reverse order of topological sort
- Only one pass through vertices required
- $\mathrm{O}(\mathbf{n}+\mathbf{m})$ time


