CS 401

Dynamic Programming:

Knapsack / RNA Secondary Structure

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Stuff

Homework 4 will be released later today

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: OPT is { 3, 4 } with value 40.

$\boxed{W = 11}$

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.

First Attempt

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

Case 1: OPT does not select item i.

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

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

Stronger DP (New Variable)

Let $OPT(i, w)$ = Max value of subsets of items $1, \ldots, i$ of weight $\leq w$

Case 1: $OPT(i, w)$ selects item i

- In this case, $OPT(i, w) = v_i + OPT(i-1, w-w_i)$

Take best of the two

Case 2: $OPT(i, w)$ does not select item i

- In this case, $OPT(i, w) = OPT(i-1, w)$.

Therefore,

$$OPT(i, w) = \begin{cases} 0 & \text{If } i = 0 \\ OPT(i-1, w) & \text{If } w_i > w \\ \max(OPT(i-1, w), v_i + OPT(i-1, w-w_i)) & \text{o.w.,} \end{cases}$$

DP for Knapsack

```
Compute-OPT(i,w)
   if M[i,w] == empty
     if (i==0)
       M[i,w]=0
     else if (wi > w)
       M[i,w]=Comp-OPT(i-1,w)
     else
       M[i,w]= max {Comp-OPT(i-1,w), vi + Comp-OPT(i-1,w-wi)}
   return M[i, w]
```

recursive

```
for w = 0 to W
   M[0, w] = 0
for i = 1 to n
   for w = 1 to W
      if (wi > w)
         M[i, w] = M[i-1, w]
      else
         M[i, w] = max {M[i-1, w], vi + M[i-1, w-wi ]}

return M[n, W]
```

Non-recursive

DP for Knapsack

W + 1

n + 1

	0	1	2	3	4	5	6	7	8	9	10	11
ϕ	0	0	0	0	0	0	0	0	0	0	0	0
{ 1 }	0											
{ 1, 2 }	0											
{ 1, 2, 3 }	0											
{ 1, 2, 3, 4 }	0											
{ 1, 2, 3, 4, 5 }	0											

W = 11

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```
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 ]}
```

DP for Knapsack

W + 1

n + 1

	0	1	2	3	4	5	6	7	8	9	10	11
ϕ	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, 2, 3 }	0											
{ 1, 2, 3, 4 }	0											
{ 1, 2, 3, 4, 5 }	0											

W = 11

```
if (w_i > w)
  M[i, w] = M[i-1, w]
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  M[i, w] = max {M[i-1, w], v_i + M[i-1, w-w_i ]}
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DP for Knapsack

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ϕ	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								
{ 1, 2, 3 }	0	1										
{ 1, 2, 3, 4 }	0	1										
{ 1, 2, 3, 4, 5 }	0	1										

OPT: { 4, 3 }
value = 22 + 18 = 40

W = 11

```
if (wi > w)
  M[i, w] = M[i-1, w]
else
  M[i, w] = max {M[i-1, w], vi + M[i-1, w-wi ]}
```

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DP for Knapsack

W + 1 →

n + 1 ↓

	0	1	2	3	4	5	6	7	8	9	10	11
ϕ	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					
{ 1, 2, 3, 4 }	0	1										
{ 1, 2, 3, 4, 5 }	0	1										

OPT: { 4, 3 }
value = 22 + 18 = 40

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if (wi > w)
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```

DP for Knapsack

W + 1

n + 1

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φ	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		
{ 1, 2, 3, 4, 5 }	0	1										

OPT: { 4, 3 }
value = 22 + 18 = 40

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```
if (wi > w)
  M[i, w] = M[i-1, w]
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ϕ	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

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Item	Value	Weight
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```
if (wᵢ > w)
  M[i, w] = M[i-1, w]
else
  M[i, w] = max {M[i-1, w], vᵢ + M[i-1, w-wᵢ ]}
```

DP Ideas so far

- You may have to strengthen DP, equivalently the induction, i.e., you have may have to carry more information to find the Optimum.
- This means that sometimes we may have to use two dimensional or three dimensional induction
- Is this dynamic algorithm a polynomial time algorithm for knapsack?
  - No
  - For an input of N bits, W can be as large as 2^N
  - Knapsack problem is actually NP-complete

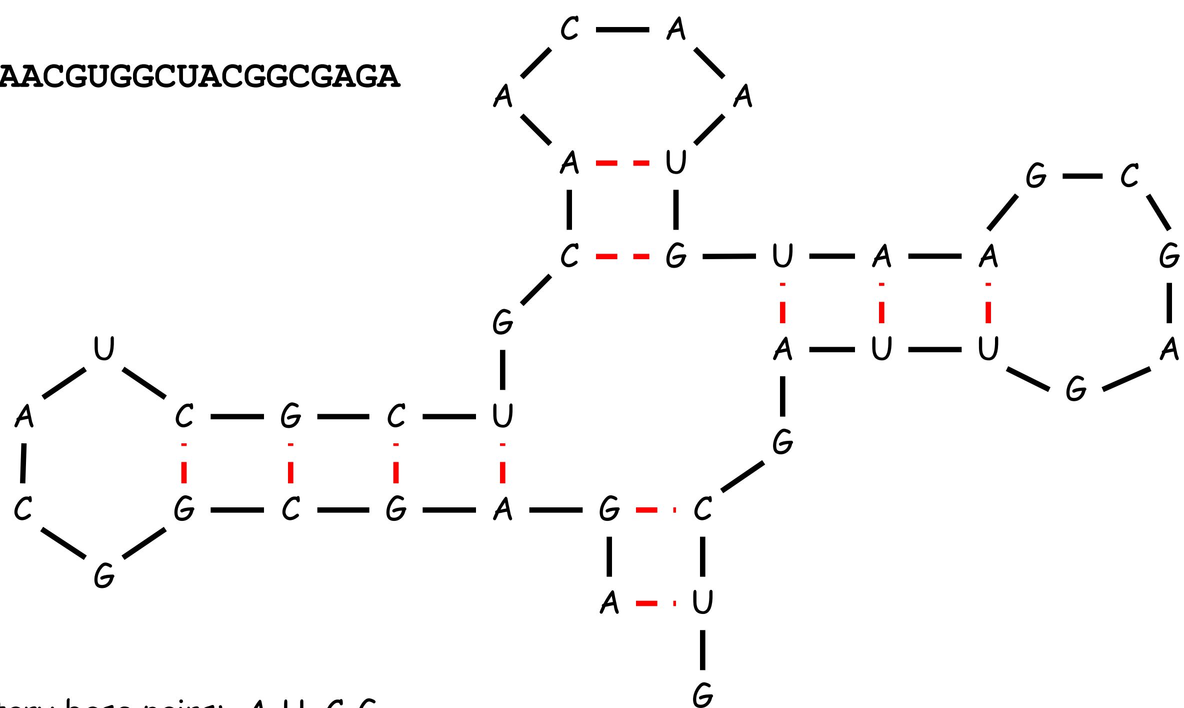
RNA Secondary Structure

RNA Secondary Structure

RNA: A 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: **GUCGAUUGAGCGAAUGUAACAACGUGGCUACGGCGAGA**



complementary base pairs: A-U, C-G

RNA Secondary Structure (Formal)

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

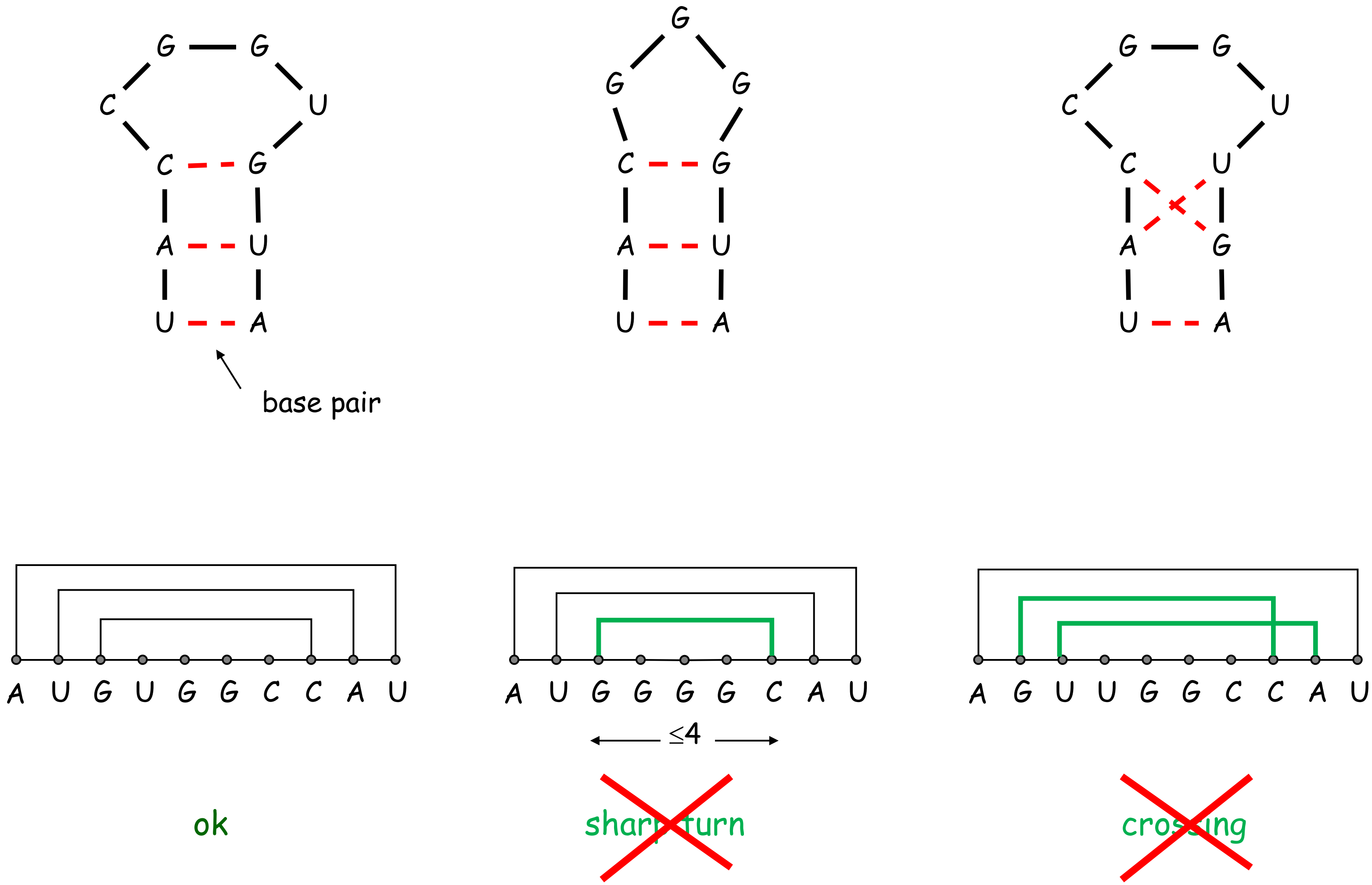
[Watson-Crick.]

- S is a *matching* and
- each pair in S is a Watson-Crick 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 $(b_i, b_j) \in S$, 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 $i < k < j < l$.

Secondary Structure (Examples)



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[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 maximize total free energy.

approximate by number of base pairs

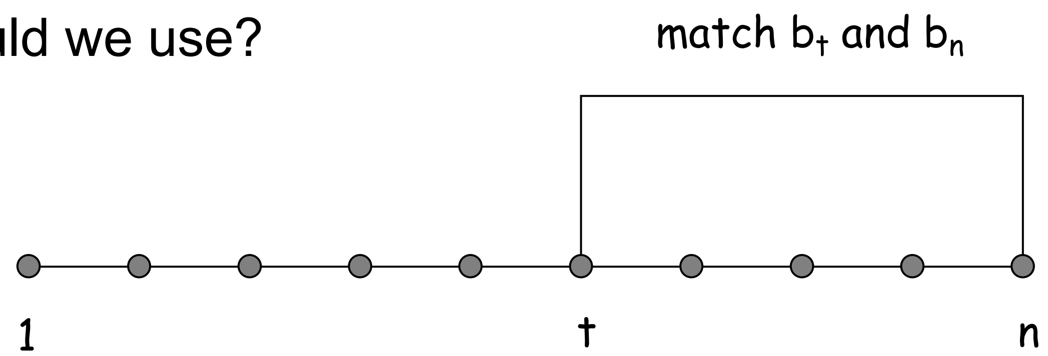
Goal: Given an RNA molecule B = $b_1 b_2 \ldots b_n$, find a secondary structure S that maximizes the number of base pairs.

DP: First Attempt

First attempt. Let $OPT(n)$ = maximum number of base pairs in a secondary structure of the substring $b_1 b_2 \ldots b_n$.

Suppose b_n is matched with b_t in $OPT(n)$.

What IH should we use?



Difficulty: This naturally reduces to two subproblems

- Finding secondary structure in $b_1, \ldots, b_{t-1}$, i.e., OPT(t-1)
- Finding secondary structure in $b_{t+1}, \ldots, b_{n-1}$,   ???

DP: Second Attempt

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

The most important part of a correct DP; It fixes IH

Case 1: If $j - i \leq 4$.

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

Case 2: Base b_j is not involved in a pair.

- $OPT(i, j) = OPT(i, j - 1)$

Case 3: Base b_j pairs with b_t for some $i \leq t < j - 4$

- non-crossing constraint decouples resulting sub-problems
- $OPT(i, j) = \max_{i \leq t < j-4} \{ 1 + OPT(i, t - 1) + OPT(t + 1, j - 1) \}$

Recursive Code

```
Let M[i,j]=empty for all i,j.

Compute-OPT(i,j){
   if (j-i <= 4)
     return 0;
   if (M[i,j] is empty)
      M[i,j]=Compute-OPT(i,j-1)
      for t=i to j-5 do
         if (b_t,b_j is in {A-U, U-A, C-G, G-C})
           M[i,j]=max(M[i,j], 1+Compute-OPT(i,t-1) +
                      Compute-OPT(t+1,j-1))
   return M[j]
}
```

Does this code terminate?
What are we inducting on?
Key question: is there any loop in the recursion?

Formal Induction

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

Base Case: $OPT(i, j) = 0$ for all i, j where $|j - i| \leq 4$.

IH: For some $\ell \geq 4$, Suppose we have computed $OPT(i, j)$ for all i, j where $|i - j| \leq \ell$.

IS: Goal: We find $OPT(i, j)$ for all i, j where $|i - j| = \ell + 1$. Fix i, j such that $|i - j| = \ell + 1$.

Case 1: Base b_j is not involved in a pair.

- $OPT(i, j) = OPT(i, j - 1)$ [this we know by IH since $|i - (j - 1)| = \ell$]

Case 2: Base b_j pairs with b_t for some $i \leq t < j - 4$

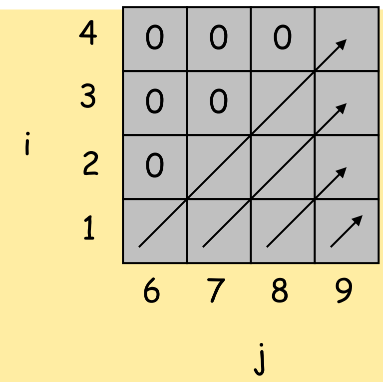
- $OPT(i, j) = \max_{i \leq t < j-4} \{ 1 + OPT(i, t - 1) + OPT(t + 1, j - 1) \}$

We know by IH since difference $\leq \ell$

Bottom-up DP

```
 for ℓ = 1, 2, …, n-1
   for i = 1, 2, …, n-1
     j = i + ℓ
     if (ℓ <= 4)
       M[i,j]=0;
       else
         M[i,j]=M[i,j-1]
         for t=i to j-5 do
           if (b_t, b_j is in {A-U, U-A, C-G, G-C})
             M[i,j]=max(M[i,j], 1+ M[i,t-1] + M[t+1,j-1])

   return M[1, n]
}
```



Running Time: $O(n^3)$

Lesson

We may not always induct on i or w to get to smaller subproblems.

We may have to induct on $|i - j|$ or $i + j$ when we are dealing with more complex problems.