Lecture 13: Dynamic Programming over Intervals

Version of March 21, 2019

Outline

1. Introduction

2. Longest Palindromic Substring

3. Optimal Binary Search trees

4. RNA Secondary Structure

DP Over Intervals

All of the problems in this lecture share the following structural properties.

- Goal is to find optimal (min or max) solution on problem with
  - Problem of size n
  - *ordered* input of items 1,2…,n
- Define substructure as
  - Ordered input of items i..j
  - Problem of size j-i+1
- Recurrence gives optimal solution of subproblem
  as function of optimal solution of smaller subproblems
- Algorithm fills in DP table from smallest to largest problem size
- Often, final subproblem filled is solution for original problem
  Sometimes, solution of original problem is min/max over table values

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Longest Palindromic Substring

Def: A palindrome is a string that reads the same backward or forward.

Ex:

- **radar, level, racecar, madam**
- "A man, a plan, a canal – Panama!" (ignoring space, punctuation, etc.)

Problem: Given a string $X = x_1 x_2 \ldots x_n$, find the longest palindromic substring.

Ex:

- $X =$ **ACCABA**
- Palindromic substrings: **CC, ACCA, ABA**
- Longest palindromic substring: **ACCA**

Note:

- Brute-force algorithm takes $O(n^3)$ time.
- Recall: A substring must be contiguous

Dynamic Programming Solution

Def: Let $p[i,j]$ be $true$ iff $X[i..j]$ is a palindrome.

The Recurrence:

Initial Conditions (subproblems of sizes 1 & 2)

- $p[i,i] = true$, **for all** i
  - **ACBBCABA**

- $p[i,i+1] = true$ **if** $x_i = x_{i+1}$
  - **ACBBCABA**

The Actual Recurrence

- $p[i,j] = true$
  if $x_i = x_j$ **AND** $p[i+1,j-1] = true$
  - **ACBBCABA**
  - **ACBBCABA**

i	1	2	3	4	5	6	7	8
	B	A	B	B	C	C	C	B

A Completed DP Table

Initial Condition
j=i; j=i+1

i/j	1	2	3	4	5	6	7	8
1	T	F						
2		T	F					
3			T	T				
4				T	F			
5					T	T		
6						T	T	
7							T	F
8								T

j=i+2

i/j	1	2	3	4	5	6	7	8
1	T	F	T					
2		T	F	F				
3			T	T	F			
4				T	F	F		
5					T	T	T	
6						T	T	F
7							T	F
8								T

j=i+3

i/j	1	2	3	4	5	6	7	8
1	T	F	T	F				
2		T	F	F	F			
3			T	T	F	F		
4				T	F	F	F	
5					T	T	T	F
6						T	T	F
7							T	F
8								T

j=i+4

i/j	1	2	3	4	5	6	7	8
1	T	F	T	F	F			
2		T	F	F	F	F		
3			T	T	F	F	F	
4				T	F	F	F	T
5					T	T	T	F
6						T	T	F
7							T	F
8								T

j>i+4

i/j	1	2	3	4	5	6	7	8
1	T	F	T	F	F	F	F	F
2		T	F	F	F	F	F	F
3			T	T	F	F	F	F
4				T	F	F	F	T
5					T	T	T	F
6						T	T	F
7							T	F
8								T

Largest is BCCCB

The Algorithm

```
max ← 1
for i ← 1 to n − 1 do                          initial conditions
    p[i,i] ← true                              j=i
    if x_i = x_{i+1} then
        p[i,i+1] ← true, max ← 2               j=i+1
    else p[i,i+1] ← false
for l ← 3 to n do
    for i ← 1 to n − l + 1 do                  j=i + (l-1)
        j ← i + l − 1
        if p[i+1,j−1] = true and x_i = x_j then
            p[i,j] ← true, max ← l
        else p[i,j] ← false
return max
```

Running time: $O(n^2)$

Space: $O(n^2)$ but can be improved to $O(n)$

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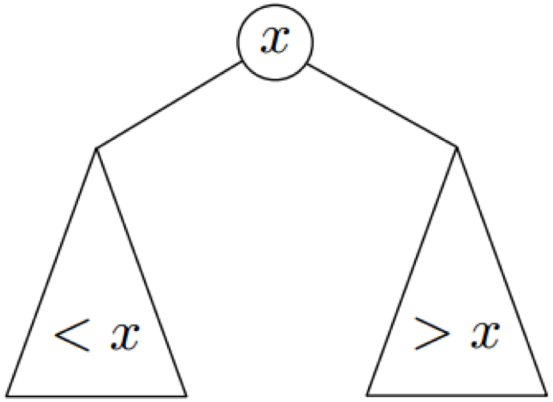
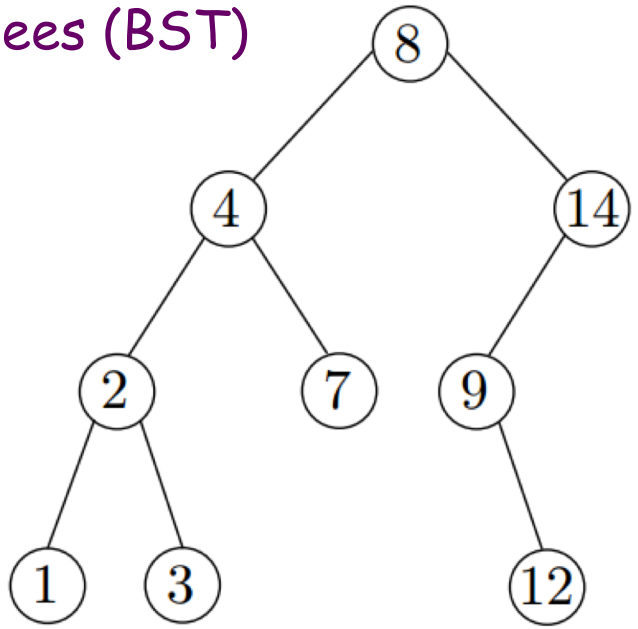
Binary search trees (BST)





Tree-Search(T, k)**:**

$x \leftarrow T.root$

while $x \neq nil$ **and** $k \neq x.key$ **do**

  if $k < x.key$ **then** $x \leftarrow x.left$

  else $x \leftarrow x.right$

return x

The (worst-case) search time in a balanced BST is $\Theta(\log n)$

Q: If we know the probability of each key being searched for, can we design a (possibly unbalanced) BST to optimize the expected search time?

The Optimal Binary Search Tree Problem

Problem Definition (simpler than the version in textbook):
Given n keys $a_1 < a_2 < \cdots < a_n$, with weights $f(a_1), \ldots, f(a_n)$, find a binary search tree T on these n keys such that

$$B(T) = \sum_{i=1}^{n} f(a_i)(d(a_i) + 1)$$

is minimized, where $d(a_i)$ is the depth of a_i.

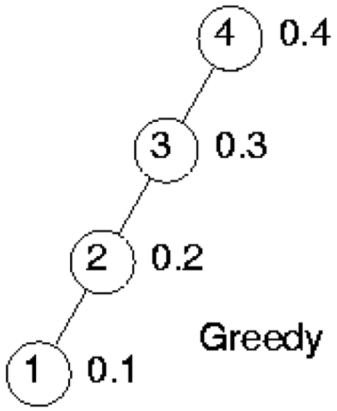
Note: Similar to the Huffman coding problem but with 2 key differences:

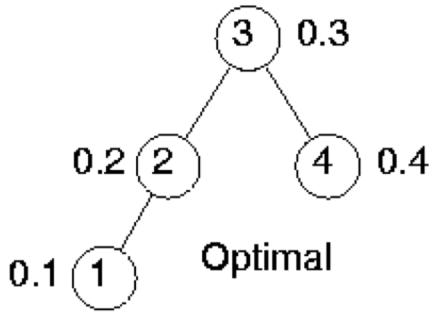
- The tree has to be a BST, i.e., the keys are stored in sorted order. In a Huffman tree, there is no ordering among the leaves.
- Keys appear as both internal and leaf nodes. In a Huffman tree, keys (characters) appear only at the leaf nodes.

Motivation: If the weights are the probabilities of the elements being searched for, such a BST will minimize the expected search cost.

Greedy Won't Work

Greedy strategy: Always pick the heaviest key as root, then recursively build the tree top-down.





$$B(T) = 0.4 \cdot 2 + 0.3 \cdot 1 + 0.2 \cdot 2 + 0.1 \cdot 3 = 1.8$$

$$B(T) = 0.4 \cdot 1 + 0.3 \cdot 2 + 0.2 \cdot 3 + 0.1 \cdot 4 = 2$$

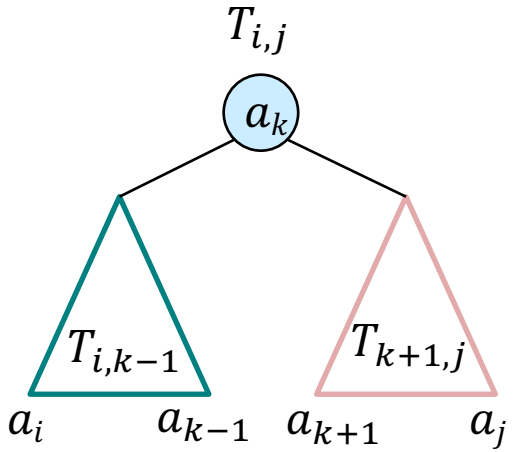
Dynamic Programming: The Recurrence

Let $T_{i,j}$ be some tree on the subset of nodes $a_i < a_{i+1} < \cdots < a_j$.
The cost is well defined as $B(T_{i,j}) = \sum_{t=i}^{j} f(a_t)(d(a_t) + 1)$

Let $w[i,j] = f(a_i) + \cdots + f(a_j)$

Suppose we ***knew*** root of $T_{i,j}$ was a_k.

$T_{i,j}$ is a BST, so left and right sub-tree children of a_k
are some tree $T_{i,k-1}$ on $a_i < \cdots < a_{k-1}$
and some tree $T_{k+1,j}$ on $a_{k+1} < \cdots < a_j$



Nodes in $T_{i,k-1}$ and $T_{k+1,j}$ are one level deeper in $T_{i,j}$ than in their original trees. So the cost of $T_{i,j}$ *is*

$$B(T_{i,j}) = (B(T_{i,k-1}) + w[i,k-1]) + f(a_k) + (B(T_{k+1,j}) + w[k+1,j])$$
$$= B(T_{i,k-1}) + B(T_{k+1,j}) + w[i,k-1] + f(a_k) + w[k+1,j]$$
$$= B(T_{i,k-1}) + B(T_{k+1,j}) + w[i,j]$$

A Deeper Dive

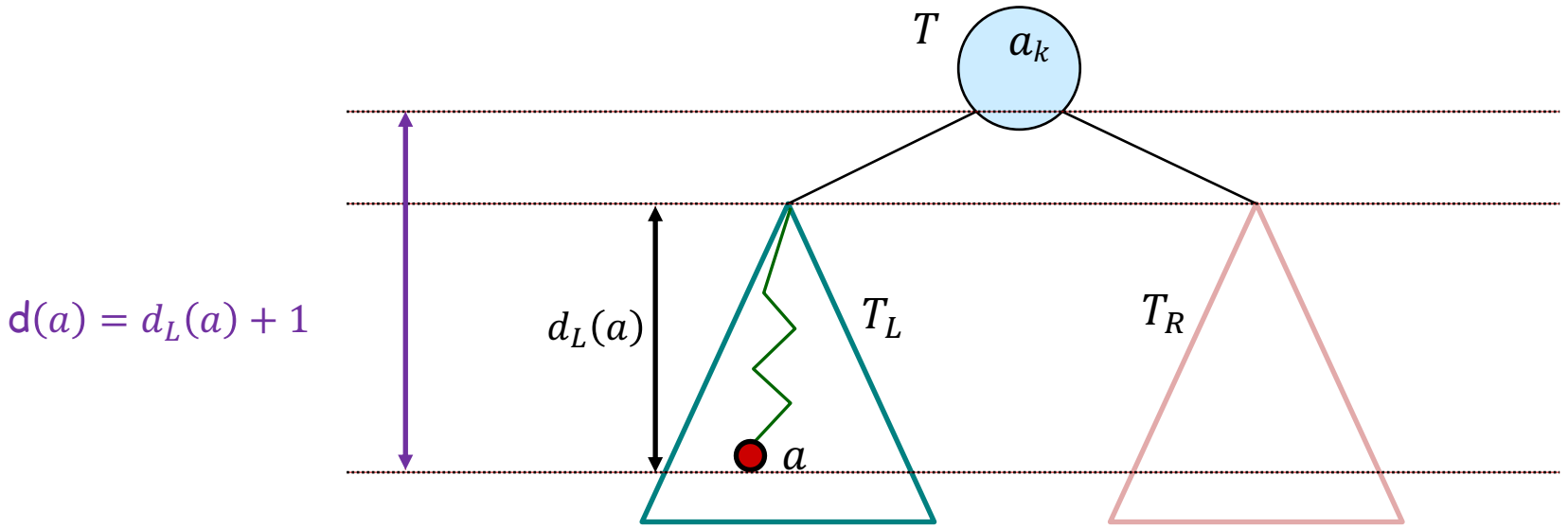
Consider a tree T_L and let $d_L(a)$ be depth of node a in tree T_L:

Now let T be a tree with root a_k & left and right subtrees T_L, T_R
Let $d(a)$ be depth of node a in tree,,

$\Rightarrow d(a) = d_L(a) + 1$

Similarly, if
$d_R(a)$ is depth of node a in tree T_R:

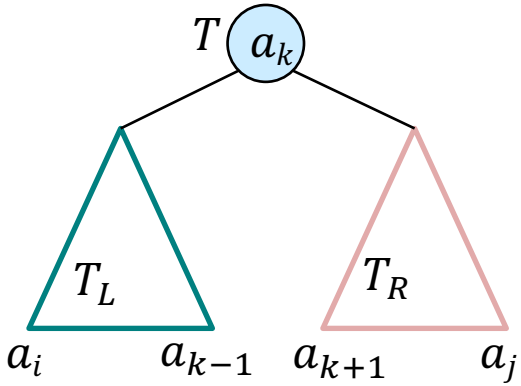
$\Rightarrow d(a) = d_R(a) + 1$



A Deeper Dive

Let T be a tree on $a_i < a_{i+1} < \cdots < a_j$
with root a_k & left and right subtrees T_L,T_R

Let $d(a)$ be depth of node a in tree,,
$d_L(a)$ be depth of node a in tree T_L: $\Rightarrow\ d(a) = d_L(a) + 1$
$d_R(a)$ be depth of node a in tree T_R: $\Rightarrow\ d(a) = d_R(a) + 1$



$w[i,j] = f(a_i) + \cdots + f(a_j)$

$$B(T) = \sum_{t=i}^{j} f(a_t)(d(a_t)+1)$$

$$= \sum_{t=i}^{k-1} f(a_t)(d(a_t)+1) + f(a_k) + \sum_{t=k+1}^{j} f(a_t)(d(a_t)+1)$$

$$= \sum_{t=i}^{k-1} f(a_t)(d_L(a_t)+1+\mathbf{1}) + f(a_k) + \sum_{t=k+1}^{j} f(a_t)((d_R(a_t)+1)+\mathbf{1})$$

$$= \sum_{t=i}^{k-1} f(a_t)(d_L(a_t)+1) + \sum_{t=1}^{k-1} \boldsymbol{f(a_t)} + f(a_k) + \sum_{t=k+1}^{j} f(a_t)(d_R(a_t)+1) + \sum_{t=k+1}^{j} \boldsymbol{f(a_t)}$$

$$= \sum_{t=i}^{k-1}[f(a_t)(d_L(a_t)+1)] + \boldsymbol{w[i,k-1]} + f(a_k) + \sum_{t=k+1}^{j}[f(a_t)(d_R(a_t)+1)] + \boldsymbol{w[k+1,j]}$$

$$= B(T_L) + \boldsymbol{w[i,k-1]} + f(a_k) + B(T_R) + \boldsymbol{w[k+1,j]}$$

$$= B(T_L) + B(T_R) + \boldsymbol{w[i,k-1]} + f(a_k) + \boldsymbol{w[k+1,j]}$$

$$= B(T_L) + B(T_R) + \boldsymbol{w[i,j]}$$

Dynamic Programming: The Recurrence

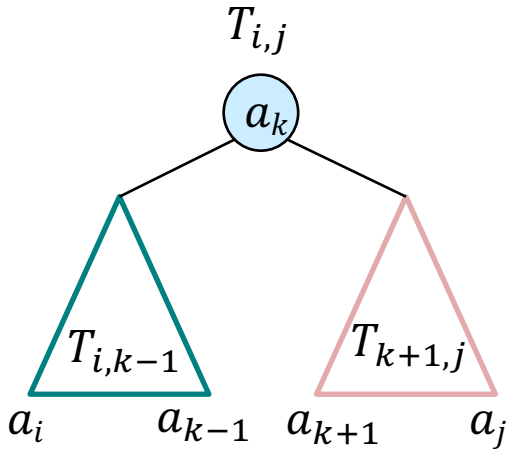
Let $T_{i,j}$ be some tree on the subset of nodes $a_i < a_{i+1} < \cdots < a_j$.
The cost is well defined as $B(T_{i,j}) = \sum_{t=i}^{j} f(a_t)(d(a_t) + 1)$

Let $w[i,j] = f(a_i) + \cdots + f(a_j)$

Suppose we ***knew*** root of $T_{i,j}$ was a_k.

The cost of $T_{i,j}$ is

$(*)\ B(T_{i,j}) = B(T_{i,k-1}) + B(T_{k+1,j}) + w[i,j].$



In particular, suppose $T_{i,j}$ has root a_k and is a minimum cost tree over all trees with nodes $a_i, \ldots, a_j$
$\Rightarrow$ its left subtree $T_{i,k-1}$ must be a minimum cost tree with nodes $a_i, \ldots, a_{k-1}$

If it wasn't, we could replace $T_{i,k-1}$ by a lesser cost subtree with nodes $a_i, \ldots, a_{k-1}$.
By (*), this would reduce $B(T_{i,j})$, contradicting that $T_{i,j}$ is a minimum cost tree.

Similarly, the right subtree $T_{k+1,j}$ must be minimum cost for $a_{k+1}, \ldots, a_j$

Dynamic Programming: The Recurrence

Def: $e[i,j]$ = the minimum cost of any BST on $a_i, \ldots, a_j$

Idea: The root of the BST can be any of $a_i, \ldots, a_j$. We try each of them.

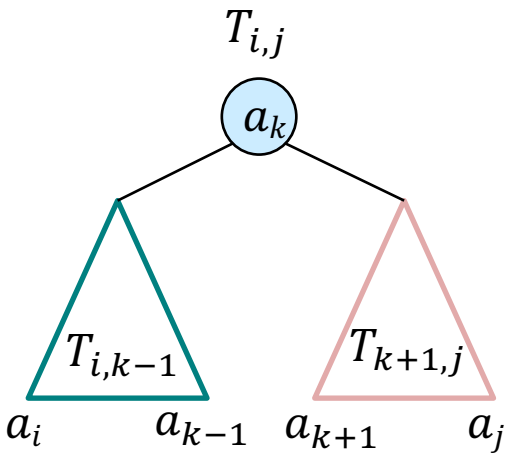
Recurrence:

Let $w[i,j] = f(a_i) + \cdots + f(a_j)$

Suppose we knew min-cost BST $T_{i,j}$ for [i,j] and that its root was a_k.

Its left subtree $T_{i,k-1}$ must be optimal for [i,k-1]
and its right subtree $T_{k+1,j}$ must be optimal for [k+1,j]

$$\Rightarrow \quad e[i,j] = B(T_{i,j})$$
$$= B(T_{i,k-1}) + B(T_{k+1,j}) + w[i,j]$$
$$= e[i,k-1] + e[k+1,j] + w[i,j]$$



To find $T_{i,j}$ we can try out every possible value of k and return the one which minimizes tree cost!

Dynamic Programming: The Recurrence

Def: $e[i,j]$ = the minimum cost of any BST on $a_i, \ldots, a_j$

Idea: The root of the BST can be any of $a_i, \ldots, a_j$. We try each of them.

Recurrence:

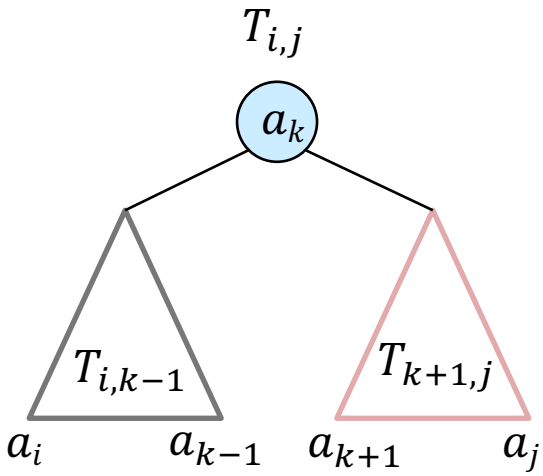
Let $w[i,j] = f(a_i) + \cdots + f(a_j)$

$$e[i,j] = \min_{i \le k \le j} \{e[i,k-1] + e[k+1,j] + w[i,j]\}$$

$e[i,j] = 0$ for $i > j$.

$e[i,i] = f(a_i)$ for all i

Note: All $w[i,j]$'s can be pre-computed in $O(n^2)$ time.



The Algorithm

Idea: We will do the bottom-up computation by the increasing order of the problem size.

```
let e[1..n, 1..n], w[1..n, 1..n], root[1..n, 1..n] be new arrays of all 0
for i = 1 to n
    w[i, i] ← f(a_i)
    for j = i + 1 to n
        w[i, j] ← w[i, j − 1] + f(a_j)
for l ← 1 to n                                          length of [i,j]
    for i ← 1 to n − l + 1
        j ← i + l − 1
        e[i, j] ← ∞
        for k ← i to j                                  Find k that
            t ← e[i, k − 1] + e[k + 1, j] + w[i, j]     minimizes
            if t < e[i, j] then                         e[i, k − 1] + e[k + 1, j] + w[i, j]
                e[i, j] ← t
                root[i, j] ← k
return Construct-BST(root, 1, n)
```

Running time: $O(n^3)$

Space: $O(n^2)$

Construct the Optimal BST

```
Construct-BST(root, i, j) :
if i > j then return nil
create a node z
z.key ← a[root[i, j]]
z.left ← Construct-BST(root, i, root[i, j] − 1)
z.right ← Construct-BST(root, root[i, j] + 1, j)
return z
```

Running time of this part: $O(n)$

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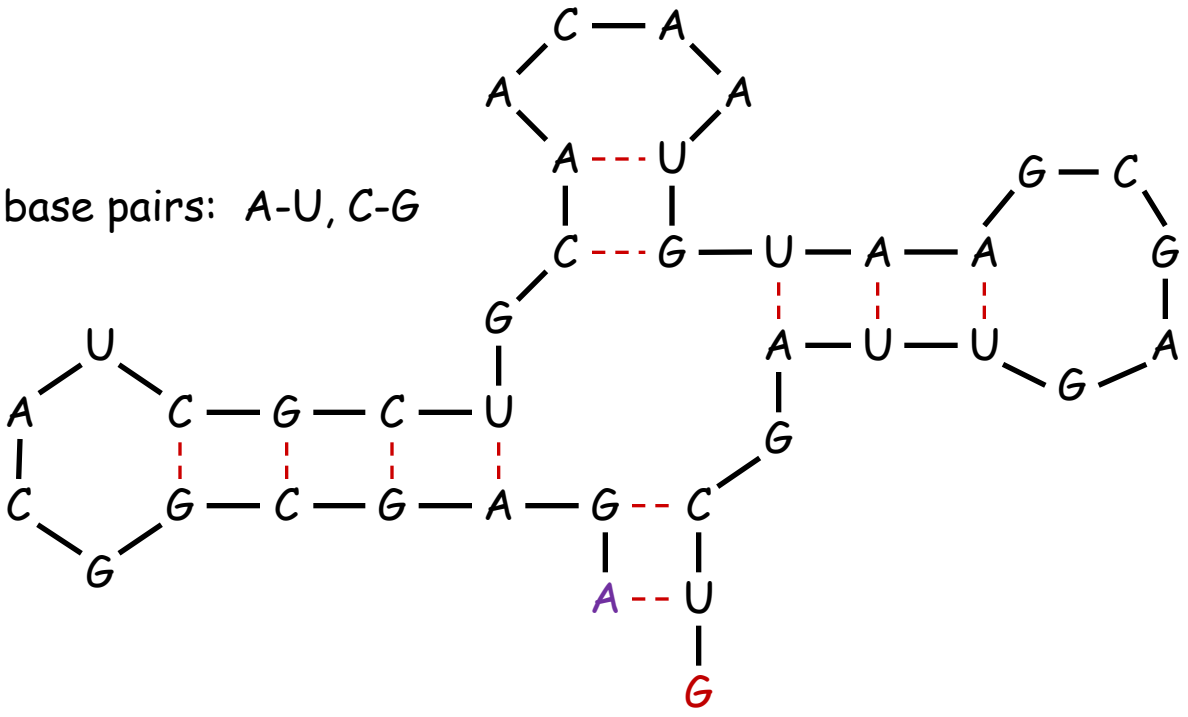
RNA Secondary Structure

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 the behavior of molecules.

Ex: GUCGAUUGAGCGAAUGUAACAACGUGGCUACGGCGAGA

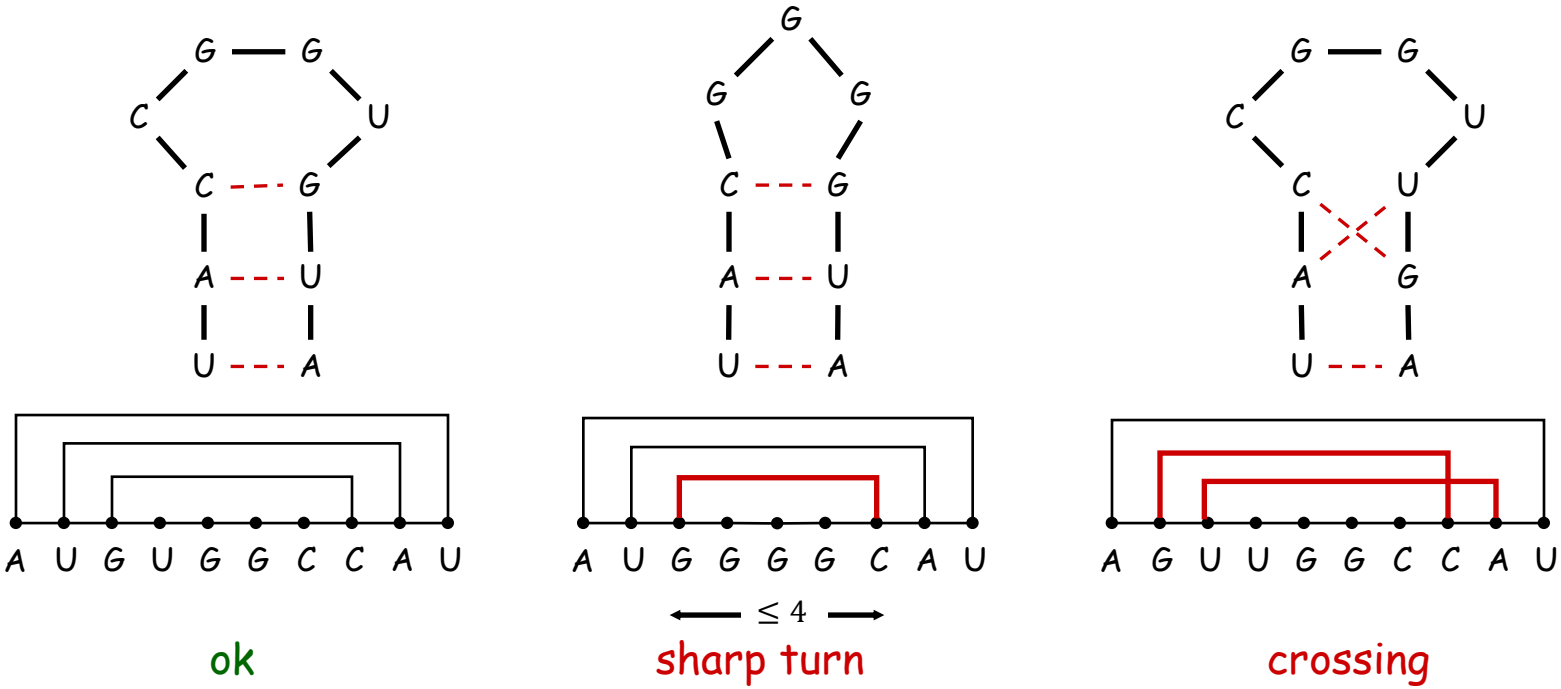
complementary base pairs: A-U, C-G



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 $i < k < j < l$.



The Problem

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

That is, find the maximum number of base pairs that can be matched satisfying the no sharp turns and no crossing constraints

The Recurrence

Def. $M[i,j]$ = maximum number of base pairs in a secondary structure of the substring $b_i b_{i+1} \ldots b_j$.

Recurrence.

- Case 1. If $i \geq j - 4$.
  - $M[i,j] = 0$ by no-sharp turns condition.

- Case 2. i< j-4

  - Case 2a: Base b_j is not matched in optimal solution for [i,j]
    - $M[i,j] = M[i,j-1]$

  - Case 2b: Base b_j pairs with b_k for some $i \leq k \leq j - 5$.
    - Try matching b_j to all possible b_k.
    - non-crossing constraint decouples problem into sub-problems
    - $M[i,j] = 1 + \max_k \{M[i,k-1] + M[k+1,j-1]\}$

Take max over k such that $i \leq k \leq j - 5$ and b_k and b_j are Watson-Crick complements

The Algorithm

```
let M[1..n, 1..n], s[1..n, 1..n] be new arrays of all 0
for l ← 1 to n
    for i ← 1 to n − l + 1
        j ← i + l − 1
        M[i, j] ← M[i, j − 1]
        for k ← i to j − 5
            if b_k and b_j are not complements then continue
            t ← 1 + M[i, k − 1] + M[k + 1, j − 1]
            if t > M[i, j] then
                M[i, j] ← t
                s[i, j] ← k
Construct-RNA(s, 1, n)
```

Running time: $O(n^3)$

Space: $O(n^2)$

```
Construct-RNA(s, i, j):
if i ≥ j − 4 then return
if s[i, j] = 0 then Construct-RNA(s, i, j − 1)
print s[i, j], "-", j
Construct-RNA(s, i, s[i, j] − 1)
Construct-RNA(s, s[i, j] + 1, j − 1)
```