## CS3000: Algorithms \& Data Jonathan Ullman

Lecture 8:

- Dynamic Programming: RNA Folding, Practice

Feb 3, 2020

## RNA Folding

## DNA

- DNA is a string of four bases $\{\mathbf{A}, \mathbf{C}, \mathbf{G}, \mathrm{T}\}$
- Two complementary strands of DNA stick together and form a double helix
- A-T and C-G are complementary pairs



## RNA Folding

- RNA is a string of four bases $\{\mathbf{A}, \mathbf{C}, \mathbf{G}, \mathrm{U}\}$
- A single RNA strand sticks to itself and folds into complex structures
- A-U and C-G are complementary pairs



## RNA Folding

- RNA strand will try to minimize energy (form the most bonds) subject to constraints



## RNA Folding

- RNA is a string of bases $\boldsymbol{b}_{\mathbf{1}}, \ldots, \boldsymbol{b}_{\boldsymbol{n}} \in\{\boldsymbol{A}, \boldsymbol{C}, \boldsymbol{G}, \boldsymbol{U}\}$
- The structure is given by a set of bonds $S$ consisting of pairs $(i, j)$ with $i<j$
- (Complements) Only $A-U$ or $C-G$ can be paired
- (Matching) No base $b_{i}$ is in two pairs in $S$
- (No Sharp Turns) If $(i, j) \in S$, then $i<j-4$
- (Non-Crossing) If $(i, j),(k, \ell) \in S$ then it cannot be the case that $i<k<j<\ell$


## RNA Folding

- Input: RNA sequence $\boldsymbol{b}_{\mathbf{1}}, \ldots, \boldsymbol{b}_{\boldsymbol{n}} \in\{A, C, G, U\}$
- Output: A set of pairs $S \subseteq\{1, \ldots, n\} \times\{1, \ldots, n\}$
- Goal: maximize the size of $S$
- (Complements) Only $A-U$ or $C-G$ can be paired
- (Matching) No base $b_{i}$ is in two pairs in $S$
- (No Sharp Turns) If $(i, j) \in S$, then $i<j-4$
- (Non-Crossing) If $(i, j),(k, \ell) \in S$ then it cannot be the case that $i<k<j<\ell$


## Dynamic Programming

- Let $O$ be the optimal set of pairs for $b_{1} \cdots b_{n}$
- Case 1: $O$ does not include any pair involving $n$
- Case 2: $O$ has $n$ pair with some $t<n-4$ in $O$



## Dynamic Programming

- Let $O_{i, j}$ be the optimal set of pairs for $b_{i} \cdots b_{j}$
- Case 1: $O_{i, j}$ does not include any pair involving $j$
- Case 2: $O_{i, j}$ has $j$ pair with some $t<j-4$ in $O$



## Dynamic Programming

- Let $\operatorname{OPT}(i, j)$ be the opt. number of pairs for $b_{i} \cdots b_{j}$
- Case 1: $j$ pairs with nothing
- Case 2: $j$ pairs with $t<j-4$



## Dynamic Programming

- Let OPT $(i, j)$ be the opt. number of pairs for $b_{i} \cdots b_{j}$
- Case 1: $j$ pairs with nothing
- Case 2: $j$ pairs with $t<j-4$

Recurrence:
OPT( $i, j$ )
$=\max \{\operatorname{OPT}(i, j-1), \max \{\operatorname{OPT}(i, t-1)+\operatorname{OPT}(t+1, j-1)\}\}$

Maximum over all $t$ such that

- $i \leq t<j-4$

Base Cases:

- $b_{t}, b_{j}$ are compatible bases
$\mathrm{OPT}(i, j)=0$ if $i \geq j-4$


## Filling the Table

Sequence: ACCGGUAGU
Recurrence:
$\operatorname{OPT}(i, j)=\max \left\{\operatorname{OPT}(i, j-1), \max _{\text {allowable }}\{\operatorname{OPT}(i, t-1)+\operatorname{OPT}(t+1, j-1)\}\right\}$

|  | 6 | 7 | 8 | $j=9$ |
| :---: | :---: | :---: | :---: | :---: |
| 4 | 0 | 0 | 0 |  |
| 3 | 0 | 0 |  |  |
| 2 | 0 |  |  |  |
| $i=1$ |  |  |  |  |

## RNA Folding Summary

- Compute the optimal RNA folding in time $O\left(n^{3}\right)$ and space $O\left(n^{2}\right)$
- Dynamic Programming:
- Decide on an optimal pair $b_{t}-b_{n}$
- Remaining RNA is two non-overlapping pieces
- Adding variables: one subproblem for each interval
- Non-crossing is critical
- Think about how the dynamic programming algorithm changes if we remove each of the conditions


## Dynamic Programming Practice



Midterm I Review

## Midterm I Topics

- Fundamentals:
- Induction
- Asymptotics
- Recurrences
- Stable Matching
- Divide and Conquer
- Dynamic Programming


## Topics: Induction

- Proof by Induction:
- Mathematical formulas, e.g. $\sum_{i=1}^{n} i=\frac{n(n+1)}{2}$
- Spot the bug
- Solutions to recurrences
- Correctness of divide-and-conquer algorithms
- Good way to study:
- Lehman-Leighton-Meyer, Mathematics for CS
- Review divide-and-conquer in Kleinberg-Tardos


## Practice Question: Induction

- Suppose you have an unlimited supply of 3 and 7 cent coins, prove by induction that you can make any amount $n \geq 12$.


## Topics: Asymptotics

- Asymptotic Notation
- $0, O, \omega, \Omega, \Theta$
- Relationships between common function types
- Good way to study:
- Kleinberg-Tardos Chapter 2


## Topics: Asymptotics

| Notation | means | Think... | E.g. |
| :---: | :---: | :---: | :---: |
| $f(\mathrm{n})=0(\mathrm{n})$ | $\begin{aligned} & \exists c>0, n_{0}>0, \forall n \geq n_{0}: \\ & 0 \leq f(n) \leq c g(n) \end{aligned}$ | At most " $\leq "$ | $100 \mathrm{n}^{2}=O\left(\mathrm{n}^{3}\right)$ |
| $f(n)=\Omega(g(n))$ | $\begin{aligned} & \exists c>0, n_{0}>0, \forall n \geq n_{0}: \\ & 0 \leq c g(n) \leq f(n) \end{aligned}$ | At least " $\geq$ " | $2^{n}=\Omega\left(n^{100}\right)$ |
| $f(\mathrm{n})=\Theta(\mathrm{g}(\mathrm{n}))$ | $\begin{aligned} & f(n)=O(g(n)) \text { and } \\ & f(n)=\Omega(g(n)) \end{aligned}$ | Equals "=" | $\log (\mathrm{n}!)=\Theta(\mathrm{n} \log \mathrm{n})$ |
| $f(n)=0(g(n))$ | $\begin{gathered} \forall c>0, \exists n_{0}>0, \forall n \geq n_{0} \\ 0 \leq f(n)<c g(n) \end{gathered}$ | Less than "<" | $\mathrm{n}^{2}=0\left(2^{n}\right)$ |
| $f(n)=\omega(\mathrm{g}(\mathrm{n}))$ | $\begin{gathered} \forall c>0, \exists n_{0}>0, \forall n \geq n_{0}: \\ 0 \leq c g(n)<f(n) \end{gathered}$ | Greater than ">" | $n^{2}=\omega(\log n)$ |

## Topics: Asymptotics

- Constant factors can be ignored
- $\forall C>0 \quad C n=O(n)$
- Smaller exponents are Big-Oh of larger exponents
- $\forall a>b \quad n^{b}=O\left(n^{a}\right)$
- Any logarithm is Big-Oh of any polynomial
- $\forall a, \varepsilon>0 \quad \log _{2}^{a} n=O\left(n^{\varepsilon}\right)$
- Any polynomial is Big-Oh of any exponential
- $\forall a>0, b>1 \quad n^{a}=O\left(b^{n}\right)$
- Lower order terms can be dropped
- $n^{2}+n^{3 / 2}+n=O\left(n^{2}\right)$


## Practice Question: Asymptotics

- Put these functions in order so that $f_{i}=O\left(f_{i+1}\right)$
- $n^{\log _{2} 7}$
- $8^{\log _{2} n}$
- $2^{3 \log _{2} \log _{2} n}$
- $2^{\left(\log _{2} n\right)^{2}}$
- $\sum_{i=1}^{n} i$
- $n^{2} \log _{2} n$


## Practice Question: Asymptotics

- Suppose $f_{1}=O(g)$ and $f_{2}=O(g)$. Prove that $f_{1}+f_{2}=O(g)$.


## Topics: Recurrences

- Recurrences
- Representing running time by a recurrence
- Solving common recurrences
- Master Theorem
- Good way to study:
- Erickson book
- Kleinberg-Tardos divide-and-conquer chapter


## Practice Question: Recurrences

```
F(n):
    For i = 1,\ldots,n': Print "Hi"
    For i = 1,\ldots,3: F(n/3)
```

- Write a recurrence for the running time of this algorithm. Write the asymptotic running time given by the recurrence.


## Topics: Recurrences

- Consder the recurrence $T(n)=\sqrt{n} \cdot T(\sqrt{n})+n$ with $T(1)=1$. Solve using a recursion tree.


## Topics: Divide-and-Conquer

- Divide-and-Conquer
- Writing pseudocode
- Proving correctness by induction
- Analyzing running time via recurrences
- Examples we've studied:
- Mergesort, Binary Search, Karatsuba's, Selection
- Good way to study:
- Example problems from Kleinberg-Tardos or Erickson
- Practice, practice, practice!


## Topics: Dynamic Programming

- Dynamic Programming
- Identify sub-problems
- Write a recurrence, $\operatorname{OPT}(n)=\max \left\{v_{n}+O P T(n-6), O P T(n-1)\right\}$
- Fill the dynamic programming table
- Find the optimal solution
- Analyze running time
- Good way to study:
- Example problems from Kleinberg-Tardos or Erickson
- Practice, practice, practice!


## Practice Question

- Design an $O(n)$-time algorithm that takes an array $A[1: n]$ and returns a sorted array containing the smallest $\sqrt{n}$ elements of $A$


## Practice Question

- Consider the following sorting algorithm

```
A[1:n] is a global array
SillySort(1,n):
    if (n <= 2): put A in order
    else:
        SillySort(1,2n/3)
    SillySort(n/3,n)
    SillySort(1,2n/3)
```

- Prove that it is correct
- Analyze its running time


## Dynamic Programming Practice



## Chocolate Bar Splitting

- Input: A chocolate bar with $n \times m$ pieces
- Output: The minimum number of cuts needed to divide the block into perfect squares


Chocolate Bar Splitting


## Vankin’s Mile

| -1 | 7 | -8 | 10 | -5 |
| ---: | ---: | ---: | ---: | ---: |
| -4 | -9 | 8 | -6 | 0 |
| 5 | -2 | -6 | -6 | 7 |
| -7 | 4 | 7 | 7 | -3 |
|  | -3 |  |  |  |
| 7 | 1 | -6 | 4 | -9 |

- Input: An $n \times n$ board of numbers
- Rules:
- Place a chip on the board
- Keep moving the tile down or right until you fall off
- Score = sum of the numbers your chip visited
- Output: The best possible strategy

