## Comp 555 - BioAlgorithms - Spring 2021


"Really? - my people always say multiply and conquer."

Divide and Conquer Algorithms

## Embedded subsequences... a hint



## Embedded subsequence:

- "No symbol can match itself"
- In other words, you can't use edges on the main diagonal

$$
\begin{array}{ll}
0,5, \mathrm{~T} & 1,3, \mathrm{~A} \\
1,6, \mathrm{~A} & 3,6, \mathrm{~A} \\
\underline{2}, 8, \mathrm{G} & 6,7, \mathrm{~A}
\end{array}
$$

## The Essence of Divide and Conquer

- Divide problem into sub-problems
- Conquer by solving sub-problems recursively.
- If the sub-problems are small enough, solve them in brute force fashion
- Combine the solutions of sub-problems into a solution of the original problem
- This is the tricky part



## Divide and Conquer Applied to Sorting

## Problem

- Given an unsorted array of items


## $\begin{array}{llllllll}5 & 2 & 4 & 7 & 1 & 3 & 2 & 6\end{array}$

- Reorder them such that they are in a non-decreasing order

$$
\begin{array}{llllllll}
1 & 2 & 2 & 3 & 4 & 5 & 6 & 7
\end{array}
$$

## Merge Sort

## Step 1. The Divide Phase


$\log _{2}(n)$ divisions to split an array of size n into single elements

## Merge Sort

## Merging

- 2 arrays of size 1 can be easily merged to form a sorted array of size 2

- Move the smaller first value of the two arrays to the next slot in the merged array. Repeat.
- 2 sorted arrays of size $p$ and $q$ can be merged in $O(p+q)$ time to form a sorted array of size $p+q$


## Merge Sort

Step 2. Conquer Phase

$O(n) \downarrow$
$\downarrow$

| 2 | 4 | 5 | 7 | 1 | 2 | 3 | 6 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |

$\log _{2}(n)$ iterations, each iteration takes $O(n)$ time, for a total time $O\left(n \log _{2}(n)\right)$

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## Now back to Biology

## All algorithms for aligning a pair of sequences thus far have required quadratic memory

The tables used by the dynamic programming method

- Space complexity for computing alignment path for sequences of length $n$ and $m$ is $O(n m)$
- We kept a table of all scores and arrival directions in memory to reconstruct the final best path (backtracking)



## Computing Alignments with Linear Memory



- If appropriately ordered, the space needed to compute just the score can be reduced to $\mathrm{O}(\mathrm{n})$
- For example, we only need the previous column to calculate the current column, and we can throw away that previous column once we're done using it


## Recycling Columns

Only two columns of scores are needed at any given time


memory for column 2 is used to calculate column 4

## An Aside

Suppose that we reverse the source and destination of our Manhattan Tour

- Does the path with the most attractions change?



## More Aside

Now suppose that we made two tours

- One from the source towards the destination
- A second from the destination of towards the source
- And we stop both tours at the middle column

- Can we combine these two separate solutions to find the overall best score?


## A Divide \& Conquer Alignment Approach



- We want to calculate the longest path from $(0,0)$ to $(\mathrm{n}, \mathrm{m})$ that passes through $(\mathrm{i}, \mathrm{m} / 2)$ where $i$ ranges from 0 to $n$ and represents the $i$-th row
- Define Score(i) as the score of the path from $(0,0)$ to $(n, m)$ that passes through vertex $(i, m / 2)$


## Finding the Midline

Define (mid,m/2) as the vertex where the best score crosses the middle column.


- How hard is the problem compared to the original DP approach?
- What does it lack?


## We know the Best Score

How do we find the best path?

- We actually know one vertex on our path, (m/2, mid).
- How do we find more?

- Hint: Knowing mid actually constrains where the paths can go


## A Mid's Mid

We can now solve for the paths from $(0,0)$ to $(\mathrm{m} / 2, \mathrm{mid})$ and $(\mathrm{m} / 2, \mathrm{mid})$ to $(\mathrm{m}, \mathrm{n})$


## And Mid-Mid's Mids (recursively)

And repeat this process until the path is from ( $\mathrm{i}, \mathrm{j}$ ) to ( $\mathrm{i}, \mathrm{j}$ )


## Algorithm's Performance

- On the first level, the algorithm fills every entry in the matrix, thus it does $\mathrm{O}(\mathrm{nm})$ work



## Work done on a second pass

- On second level, the algorithm fills half the entries in the matrix, thus it does $\mathrm{O}(\mathrm{nm}) / 2$ work



## Work done on an Alternate second pass

- This is true regardless of what mid is



## Work done on a third pass

- On the third pass, the algorithm fills a quarter of the entries in the matrix, thus it does $\mathrm{O}(\mathrm{nm}) / 4$ work



## Sum of a Geometric Series



Total Space: $\mathrm{O}(\mathrm{n})$ for score computation, $\mathrm{O}(\mathrm{n}+\mathrm{m})$ to store the optimal alignment

- Time complexity is still $O(\mathrm{mn})$. Actually, we expect it to take about twice as long as the approach using $O(m n)$ space


## Next Time

- A closer look into Protein Sequencing
- How the molecular weights of peptide sequences can be used to untangle a protein's sequence


