

Lecture 12: Divide and Conquer Algorithms

Study Chapter 7.1 – 7.4 Last lecture covered on next Wednesday's (3/4) midterm

Spring 2015

Divide and Conquer Algorithms

- **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 (tricky part)



Sorting Problem Revisited

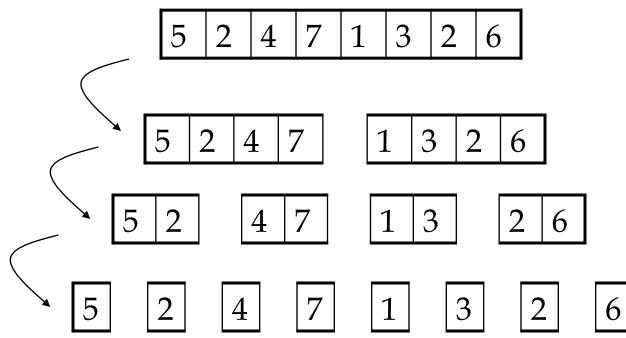
• Given: an unsorted array

• Goal: sort it



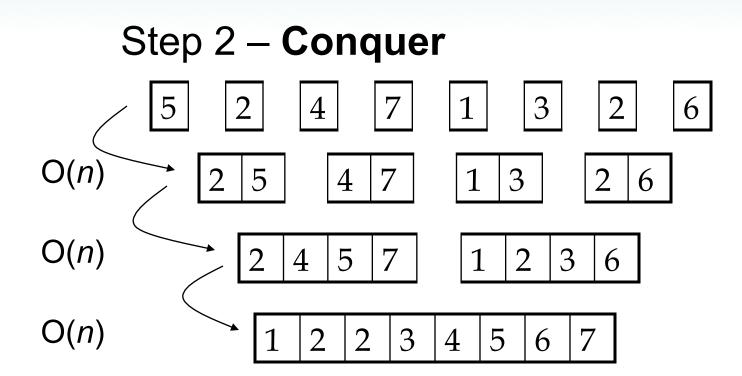
Mergesort: Divide Step

Step 1 – Divide



log(n) divisions to split an array of size n into single elements

Mergesort: Conquer Step



log *n* iterations, each iteration takes O(n) time. Total Time: $O(n \log n)$

Mergesort: Merge

Merge

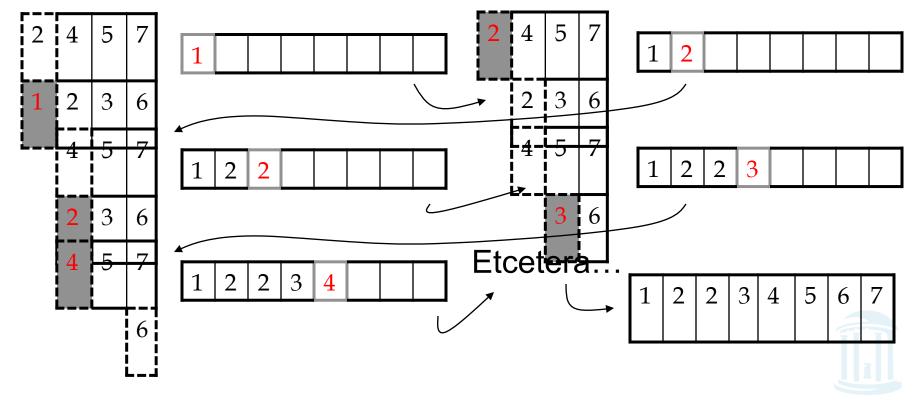
 2 arrays of size 1 can be easily merged to form a sorted array of size 2

 2 sorted arrays of size *n* and *m* can be merged in O(n+m) time to form a sorted array of size n+m



Mergesort: Merge

Merge 2 arrays of size 4



Merge Algorithm

1. <u>Merge(*a*,*b*)</u> 2. $n1 \leftarrow$ size of array a 3. $n2 \leftarrow size of array b$ 4. $a_{n1+1} \leftarrow \infty$ 5. $a_{n2+1} \leftarrow \infty$ 6. $i \leftarrow 1$ *7. j* ← 1 *8. for k* ← 1 to *n*1 + *n*2 9. *if* $a_i < b_j$ 10. $C_k \leftarrow a_i$ 11. *i* ← *i* + 1 12. *else* 13. $c_k \leftarrow b_j$ j← j+ 1 14. 15.return c



MergeSort Algorithm

1. MergeSort(*c*)

- 2. $n \leftarrow \text{size of array } c$
- *3. if n* = 1
- 4. return c
- 5. *left* \leftarrow list of first n/2 elements of c
- 6. right \leftarrow list of last n-n/2 elements of c
- 7. sortedLeft ← MergeSort(left)
- 8. sortedRight ← MergeSort(right)



MergeSort: Running Time

- The problem is simplified to baby steps
 - for the *i*'th merging iteration, the complexity of the problem is O(n)
 - number of iterations is O(log n)
 - running time: O(*n* log*n*)

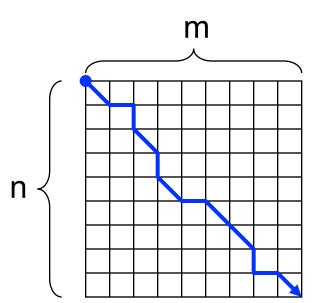
Now for a biological problem



Alignments Require Quadratic Memory

Alignment Path

- Space complexity for computing alignment path for sequences of length *n* and *m* is O(*nm*)
- We keep a table of all scores and backtracking references in memory to reconstruct the path (backtracking)

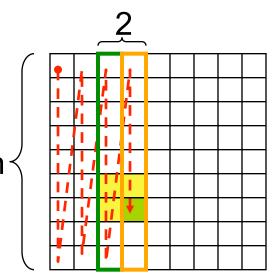




Computing Alignment Score with Linear Memory

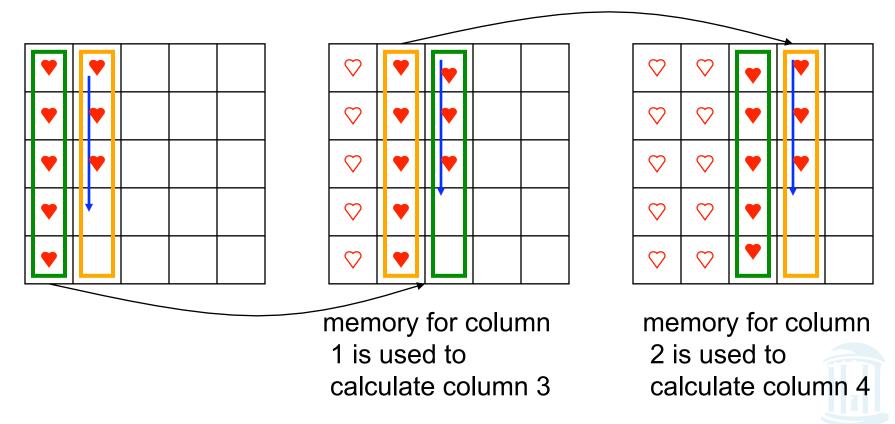
Alignment Score

- However, the space complexity of just computing the score itself is only O(n)
- For example, we only need not the previous column to calculate the current column, and we can throw away that previous column once we're done using it



Computing Alignment Score: Recycling Columns

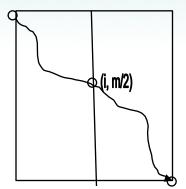
Only two columns of scores are saved at any given time



D&C Sequence Alignment

Find the best scoring path aligning two sequences

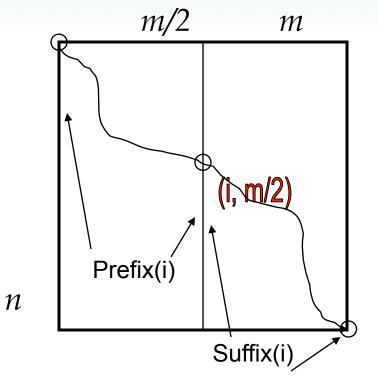
Path(source, sink)



- 1. **if**(*source* & *sink* are in consecutive columns)
- 2. output the longest path from *source* to *sink*
- 3. else
- 4. *middle* ← vertex with largest score from *source* to *sink*
- 5. Path(source, middle)
- 6. Path(middle, sink)

The only problem left is how to find this "middle vertex"!

Computing the Alignment Path



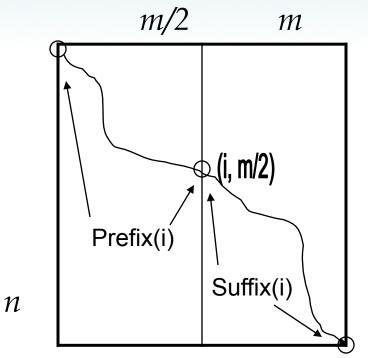
We want to calculate the longest path from (0,0) to (n,m) that passes through (i,m/2) where i ranges from 0 to *n* and represents the *i*-th row

Define

length(i)

as the length of the longest path from (0,0) to (n,m) that passes through vertex (*i*, *m*/2)

Crossing the Midline

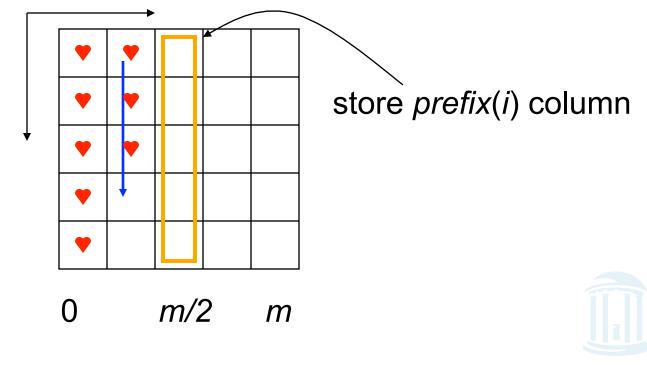


Define (*mid*,*m*/2) as the vertex where the longest path crosses the middle column.

$$length(mid) = optimal length = max_{0 \le i \le n} length(i)$$

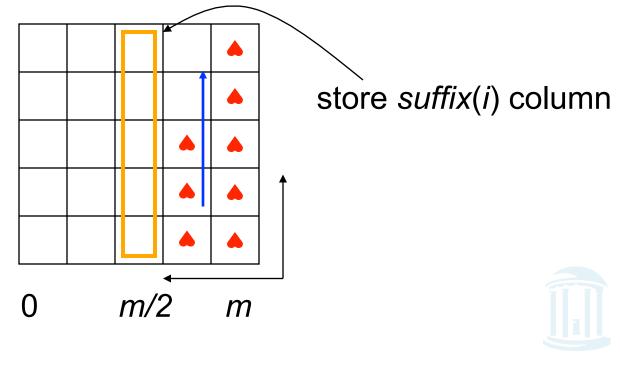
Computing Prefix(i)

- prefix(i) is the length of the longest path from (0,0) to (i,m/2)
- Compute prefix(i) in the left half of the matrix



Computing Suffix(i)

- suffix(i) is the length of the longest path from (i,m/2) to (n,m)
- suffix(i) is the length of the longest path from (n,m) to (i,m/2) with all edges reversed
- Compute *suffix(i)* in the right half of the "reversed" matrix

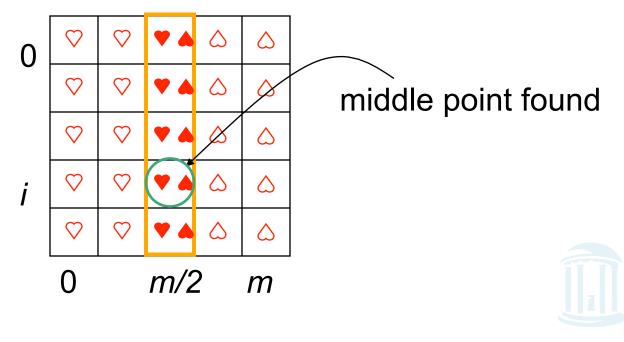


Length(i) = Prefix(i) + Suffix(i)

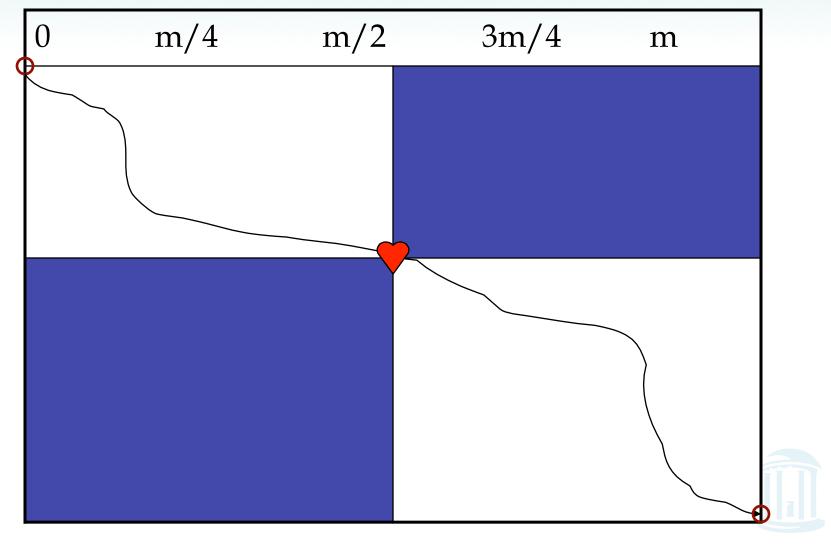
Add prefix(i) and suffix(i) to compute length(i):

length(i)=prefix(i) + suffix(i)

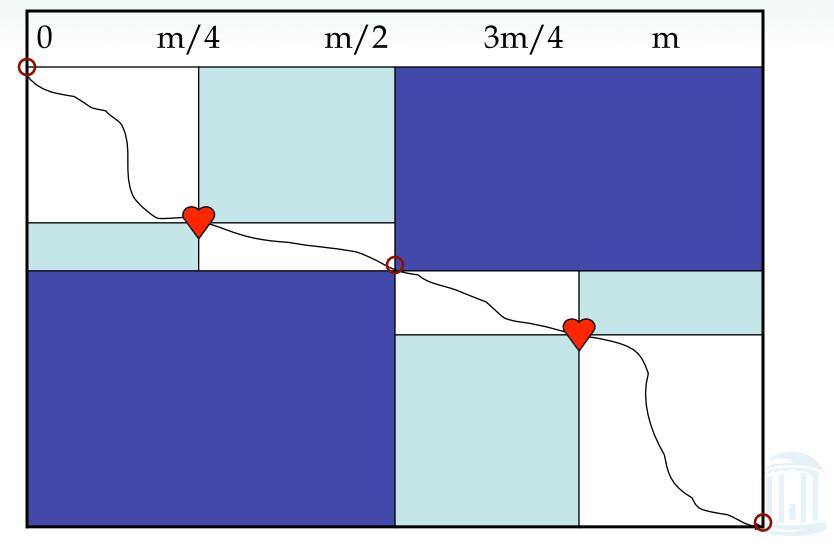
 You now have a middle vertex of the maximum path (*i*,*m*/2) as maximum of *length(i*)



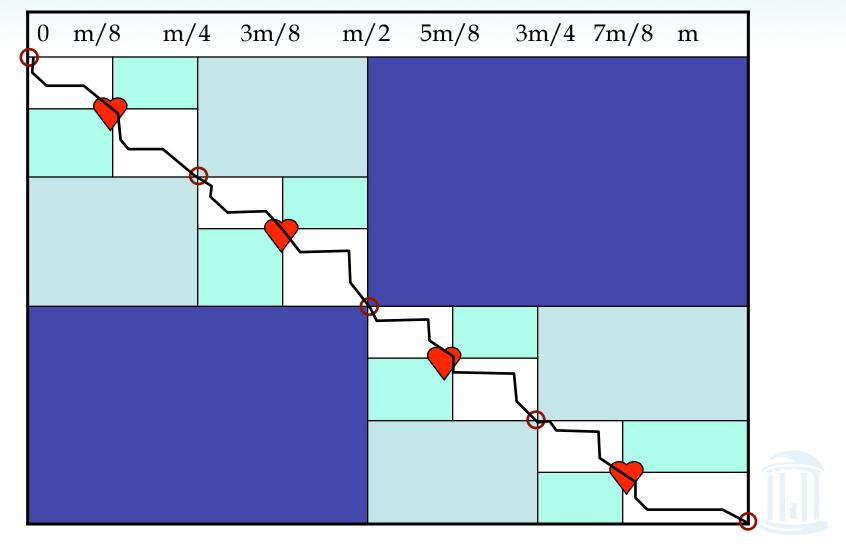
Finding the Middle Point



Finding the Middle Point again



And Again

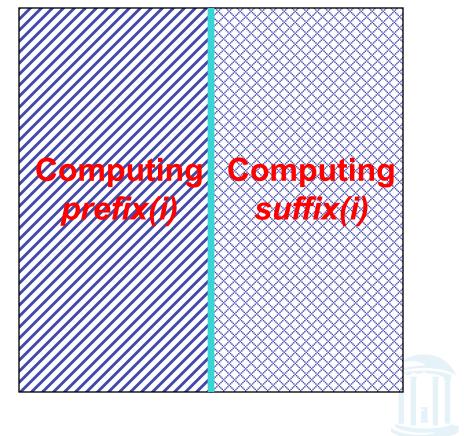


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Time = Area: First Pass

 On first level, the algorithm touches the entire area

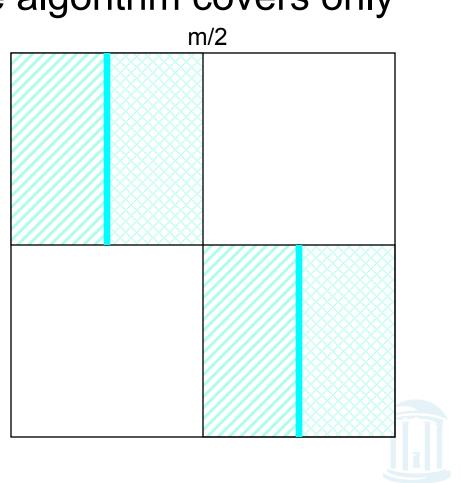
Area = n^*m



Time = Area: Second Pass

 On second level, the algorithm covers only 1/2 of the area

Area/2



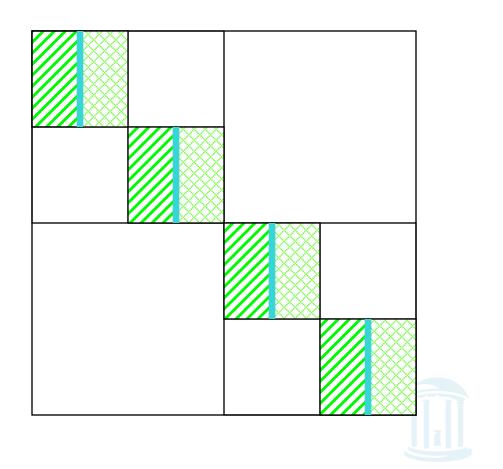
Time = Area: Second Pass

On second pass, the algorithm covers only 1/2 of the area m/2Area/2Regardless of i's value!

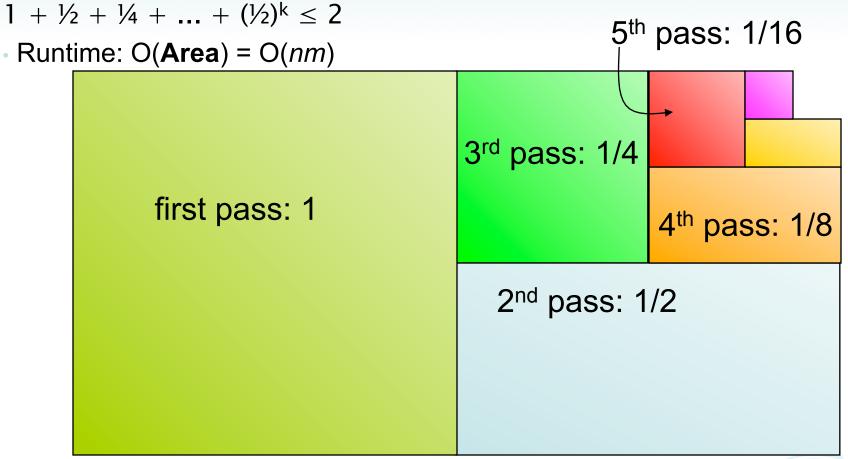
Time = Area: Third Pass

• On third pass, only 1/4th is covered.

Area/4



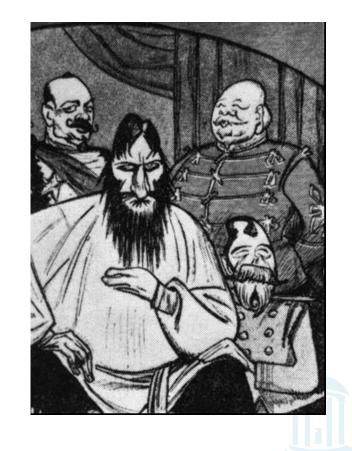
Geometric Reduction At Each Iteration



Total Space: O(n) for score computation, O(n+m) to store the optimal alignment

Can We Do Even Better?

- Align in Subquadratic Time?
- Dynamic Programming takes O(nm) for global alignment, which is quadratic assuming n ≈ m
- Yes, using the *Four-Russians Speedup*

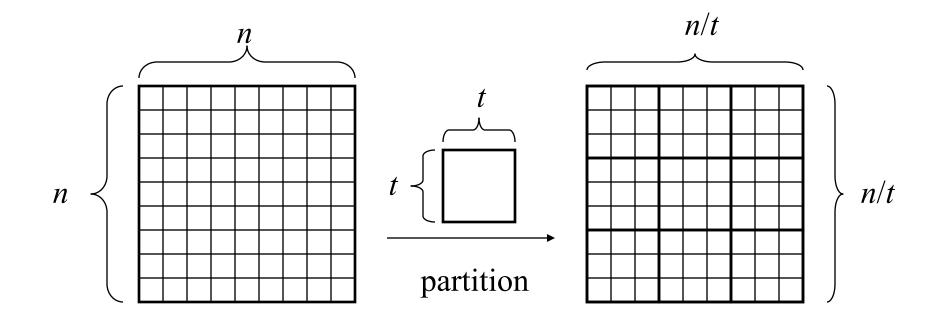


Partitioning Sequences into Blocks

- Partition the *n* x *n* grid into blocks of size *t* x *t*
- We are comparing two sequences, each of size *n*, and each sequence is sectioned off into chunks, each of length *t*
- Sequence $u = u_1...u_n$ becomes $|u_1...u_t| |u_{t+1}...u_{2t}| ... |u_{n-t+1}...u_n|$ and sequence $v = v_1...v_n$ becomes $|v_1...v_t| |v_{t+1}...v_{2t}| ... |v_{n-t+1}...v_n|$



Partitioning Alignment Grid into Blocks



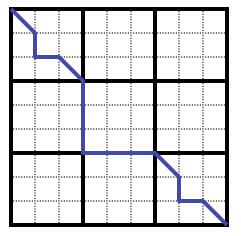
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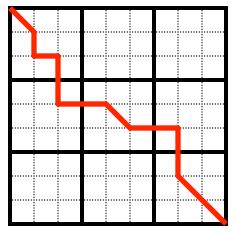
Block Alignment

- **Block alignment** of sequences *u* and *v*:
 - 1.An entire block in *u* is aligned with an entire block in *v*
 - 2. An entire block is inserted
 - 3.An entire block is deleted
- **Block path**: a path that traverses every *t* x *t* square through its corners



Block Alignment: Examples





valid

invalid



Block Alignment Problem

- <u>Goal</u>: Find the longest block path through an edit graph
- <u>Input</u>: Two sequences, *u* and *v* partitioned into blocks of size *t*. This is equivalent to an *n* x *n* edit graph partitioned into *t* x *t* subgrids
- <u>Output</u>: The block alignment of *u* and *v* with the maximum score (longest block path through the edit graph

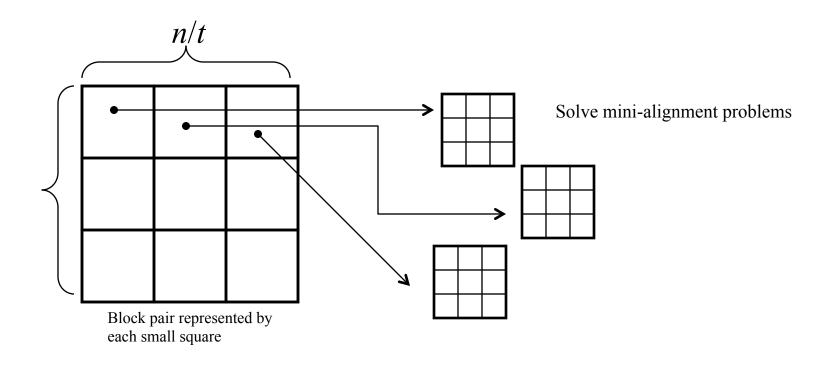


Constructing Alignments within Blocks

- To solve: compute alignment score $\beta_{i,j}$ for each pair of blocks $|u_{(i-1)*t+1}...u_{i*t}|$ and $|v_{(j-1)*t+1}...v_{j*t}|$
- How many blocks are there per sequence?
 (n/t) blocks of size t
- How many pairs of blocks for aligning the two sequences?
 - $(n/t) \ge (n/t)$
- For each block pair, solve a *mini-alignment* problem of size *t* x *t*, which requires *t* x *t* = *O*(*t*²) effort
- Looks like a wash $O((n/t)^2 t^2) = O(n^2)$, but is it?



Constructing Alignments within Blocks





Block Alignment: Dynamic Programming

 Let s_{i,j} denote the optimal block alignment score between the first *i* blocks of *u* and first *j* blocks of *v*

$$s_{i,j} = \max \begin{cases} s_{i-1,j} - \sigma_{block} \\ s_{i,j-1} - \sigma_{block} \\ s_{i-1,j-1} + \beta_{i,j} \end{cases}$$

 σ_{block} is the penalty for inserting or deleting an entire block

 $\beta_{i,j}$ is score of pair of blocks in row *i* and column *j*.



Block Alignment Runtime

- Indices *i*,*j* range from 0 to n/t
- Running time of algorithm is $O([n/t]^*[n/t]^*O(\beta_{i,j})) = O(n^2/t^2)$
- Computing all $\beta_{i,j}$ requires solving $(n/t)^*(n/t)$ mini block alignments, each of size (t^*t)
- So computing all $\beta_{i,j}$ takes time O($(n^2/t^2) t^2$) = O(n^2)
- Looks like a wash, but is it?

Recall Our Bag of Tricks

- A key insight of dynamic programming was to reuse repeated computations by storing them in a tableau
- Are there any repeated computations in Block Alignments?
- Let's check out some numbers...
 - Lets assume n = m = 4000 and t = 4
 - n/t = 1000, so there are 1,000,000 blocks
 - How many possible many blocks are there?
 - Assume we are aligning DNA with DNA, so there sequences are over an alphabet of {A,C,G,T}
 - Possible sequences are $4^t = 4^4 = 256$,
 - Possible alignments are $4^t \times 4^t = 65536$
 - There are fewer possible alignments than blocks, thus we must be frequently revisiting alignments!

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Comp 555

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Four Russians Technique

- The trick is in how to pick *t* relative to *n*
- If we pick $t = \log_2(n)/4$
- Instead of having (n/t)*(n/t) mini-alignments, construct 4^t x 4^t mini-alignments for all pairs of t nucleotide sequences, and put in a lookup table.
- However, size of lookup table is not really that huge if *t* is small.
- If $t = (\log_2 n)/4$. Then $4^t x 4^t = 4\sqrt{n^2} x \sqrt[4]{n^2} = n$



Look-up Table for Four Russians Technique

each sequence has *t* nucleotides

otides	AAAAA	AAAAC	AAAAG	AAAAT	AAAACA	
ΑΑΑΑΑ	6	4	4	4	4	
AAAAAC	4	6	4	4	3	
AAAAAG	4	4	6	4	3	
AAAAT	4	4	4	6	3	
AAAACA	4	3	3	3	6	

Lookup table "Score"

size is *n*, which is much smaller than $(n/t)^*(n/t) \rightarrow$ repeats

> Rather than precomputing this table you could actually use a hash table and compute it lazily

You can also order the sequences (alphabetize them) to exploit the symmetry, thus cutting the table-size in half

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New Recurrence

• The new lookup table *Score* is indexed by a pair of *t*-nucleotide strings, so

$$s_{i,j} = \max \begin{cases} s_{i-1,j} - \sigma_{block} \\ s_{i,j-1} - \sigma_{block} \\ s_{i-1,j-1} + Score(i^{th} block of v, j^{th} block of u) \end{cases}$$



Four Russians Speedup Runtime

- Since computing the lookup table *Score* of size *n* takes O(*n*) time, the running time is dominated by the (*n*/*t*)*(*n*/*t*) accesses to the lookup table
- Overall running time: O($[n^2/t^2]$)
- Since $t = (\log_2 n)/4$, substitute in:
- O($[n^2/\{\log_2 n\}^2]$) = O($n^2/\log(n \log n)$)



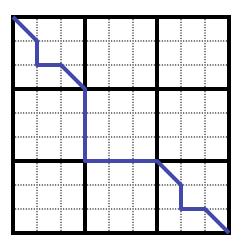
So Far...

- We can divide up the grid into blocks and run dynamic programming only on the corners of these blocks
- In order to speed up the mini-alignment calculations to under *n*², we create a lookup table of size *n*, which consists of all scores for all *t*-nucleotide pairs
- Running time goes from quadratic, O(n²), to subquadratic: O(n²/log(n log n))

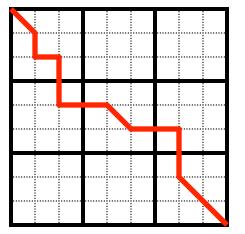


Four Russians Speedup for LCS

• Unlike the block partitioned graph, the LCS path is not restricted to pass through the vertices of the blocks.







longest common subsequence

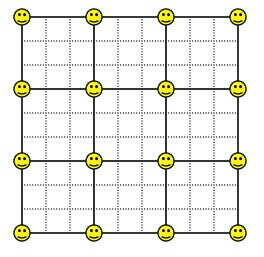


Block Alignment vs. LCS

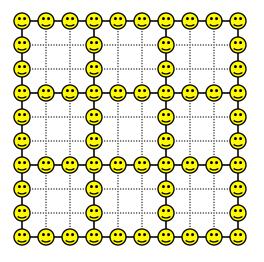
- In block alignment, we only care about the corners of the blocks.
- In LCS, we care about all points on the edges of the blocks, because those are points that the path can traverse.
- Recall, each sequence is of length *n*, each block is of size *t*, so each sequence has (*n*/*t*) blocks.



Block Alignment vs. LCS: Points Of Interest



block alignment has $(n/t)^*(n/t) = (n^2/t^2)$ points of interest



LCS alignment has $O(n^2/t)$ points of interest



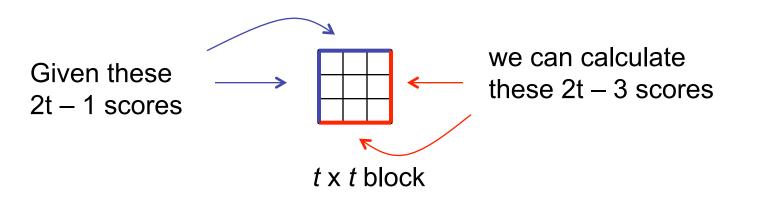
Traversing Blocks for LCS

- Given alignment scores $s_{i,*}$ in the first row and scores $s_{*,j}$ in the first column of a $t \ge t$ mini square, compute alignment scores in the last row and column of the minisquare.
- To compute the last row and the last column score, we use these 4 variables:
 - 1. alignment scores $s_{i,*}$ in the first row
 - 2. alignment scores $s_{*,i}$ in the first column
 - 3. substring of sequence u in this block (4^t possibilities)
 - 4. substring of sequence v in this block (4^t possibilities)



Traversing Blocks for LCS (cont'd)

• If we used this to compute the grid, it would take quadratic, $O(n^2)$ time, but we want to do better.





Four Russians Speedup

- Build a lookup table for all possible values of the four variables:
 - 1. all possible scores for the first row $s_{*,i}$
 - 2. all possible scores for the first column $s_{*,i}$
 - 3. substring of sequence u in this block (4^t possibilities)
 - 4. substring of sequence v in this block (4^t possibilities)
- For each quadruple we store the value of the score for the last row and last column.
- This will be a huge table, but we can eliminate alignments scores that don't make sense



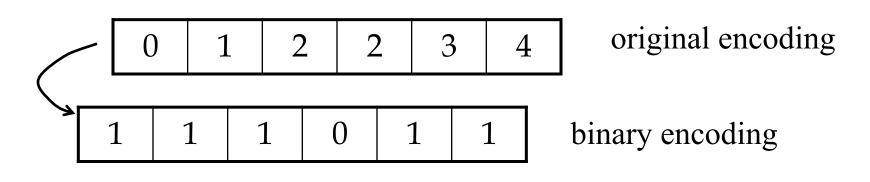
Reducing Table Size

- Alignment scores in LCS are monotonically increasing, and adjacent elements can't differ by more than 1
- Example: 0,1,2,2,3,4 is ok; 0,1,**2,4**,5,8, is not because 2 and 4 differ by more than 1 (and so do 5 and 8)
- Therefore, we only need to store quadruples whose scores are monotonically increasing and differ by at most 1



Efficient Encoding of Alignment Scores

• Instead of recording numbers that correspond to the index in the sequences *u* and *v*, we can use binary to encode the differences between the alignment scores





Reducing Lookup Table Size

- 2^t possible scores (t = size of blocks)
- 4^t possible strings
 - Lookup table size is $(2^t * 2^t)*(4^t * 4^t) = 2^{6t}$

• Let
$$t = (\log n)/4;$$

- Table size is: $2^{6((\log n)/4)} = n^{(6/4)} = n^{(3/2)}$

- Time = O($[n^2/t^2]*\log n$)
- $O([n^2/\{\log n\}^2]^*\log n) \equiv O((n^2/\log n))$



Summary

- We take advantage of the fact that for each block of $t = \log(n)$, we can pre-compute all possible scores and store them in a lookup table of size $n^{(3/2)}$
- We used the Four Russian speedup to go from a quadratic running time for LCS to subquadratic running time: $O(n^2/\log(n \log n))$
- Next Time: Graph Algorithms

