

Homework 3: due by 11:59pm on Monday, April 5, 2021

Instructor: Mack Joyner

Programming Checkpoint 1 due by 11:59pm on Monday, March 22, 2021

Total score: 100 points

All homework should be committed in the GitHub classroom repository at https://classroom.github.com/a/0Si5g_QT. In case of problems committing your files, please contact the teaching staff at comp322-staff@mailman.rice.edu before the deadline to get help resolving for your issues.

Your solution to the written assignment should be submitted as a PDF file named `hw3-written.pdf` in the `hw3` directory. This is important — you will be penalized 5 points if you place the file in some other folder or with some other name. The PDF file can be created however you choose. If you scan handwritten text, make sure that you use a proper scanner (not a digital camera) to create the PDF file. Your solution to the programming assignment should be submitted in the appropriate location in the `hw3` directory.

The slip day policy for COMP 322 is similar to that of COMP 321. All students will be given 3 slip days to use throughout the semester. When you use a slip day, you will receive up to 24 additional hours to complete the assignment. You may use these slip days in any way you see fit (3 days on one assignment, 1 day each on 3 assignments, etc.). Slip days will be tracked in Canvas.

Other than slip days, no extensions will be given unless there are exceptional circumstances (such as severe sickness, not because you have too much other work). Such extensions must be requested and approved by the instructor (via e-mail, phone, or in person) before the due date for the assignment. Last minute requests are likely to be denied.

If you see an ambiguity or inconsistency in a question, please seek a clarification on Piazza (remember not to share homework solutions in public posts) or from the teaching staff. If it is not resolved through those channels, you should state the ambiguity/inconsistency that you see, as well as any assumptions that you make to resolve it.

Finally, please note that the programming project for this homework is more challenging than in the past homework. It is important for you to start early, and to meet the intermediate checkpoint to ensure that you are on track to complete the entire homework before the final deadline.

Honor Code Policy: All submitted homework is expected to be the result of your individual effort. You are free to discuss course material and approaches to problems with your other classmates, the teaching assistants and the professor, but you should never misrepresent someone else's work as your own. If you use any material from external sources, you must provide proper attribution.

1 Written Assignments (25 points total)

Submit your solutions to the written assignments as a PDF file named `hw3_written.pdf` in the `hw3` directory. Please note that you be penalized 10 points if you misplace the file in some other folder or if you submit the report in some other format. The written portion is due along with the final submission by April 5, 2021.

1.1 Parallel Topological Sort

Recall from COMP 182 that a *directed, acyclic graph* (DAG) is a directed graph with no cycles. A *topological sort* of a DAG $g = (V, E)$ is a linear ordering of all its nodes such that if g contains an edge (u, v) , then u appears before v in the ordering. For this question, assume that the DAG is restricted so that only node 0 is a *root node* (i.e., a node with no incoming edges), and all other nodes have at least one incoming edge. Algorithm **DFS** below shows how to perform a sequential depth-first search traversal for such a DAG, which prints node indices in a preorder traversal of the DAG.

Algorithm 1: DFS of DAG with single root node

Input: Graph $g = (V, E)$, $V = \{0, 1, \dots, n - 1\}$, parent map $p_i, \forall i \in V$ (node 0 is the only root node).

Output: None.

Modifies: Parent map, p .

```
 $p_0 \leftarrow -1$  ; // We designate the parent of the root node to be '-1'  
Visit( $g, 0, p$ );
```

Algorithm 2: Visit

Input: Graph $g = (V, E)$, node $i \in V$, and $p_j, \forall j \in V$.

Output: None.

Modifies: p .

Print i ; // Use any parallel constructs that you've learned in Module 1 to ensure that these print statements are performed in a topological sort order

foreach neighbor h of i **do**

```
    if  $p_h = \text{null}$  then  
         $p_h \leftarrow i$ ;  
        Visit( $g, h, p$ );
```

- (5 points) Summarize the similarities and differences between futures and data-driven futures in HJ-lib. In your summary, you should state if it is possible to create a race condition or a deadlock when accessing the value in the future container when using either construct.
- (15 points) Modify algorithm **DFS** above by *adding parallel constructs* to ensure that the print statements occur in a *topological sort* order for the given DAG. You may add any parallel constructs that you've learned in Module 1 (e.g., async tasks, future tasks, data-driven tasks, etc.) and also add auxiliary objects as needed (e.g., futures, data-driven futures, etc.), but the basic depth-first traversal in the original algorithm cannot be modified. Explain why your modified algorithm prints the node indices in a topological sort order.
- (5 points) Explain if your modified algorithm in 1.1.2 above is guaranteed to be *functionally deterministic* and/or *structurally deterministic*, and why.

2 Programming Assignment (75 points)

2.1 Pairwise Sequence Alignment

In this homework, we will focus on the *pairwise sequence alignment* problem in evolutionary and molecular biology, and how parallelism can help in solving this problem. (This homework is adapted from a COMP 182 homework assignment by Prof. Luay Nakhleh.)

Let X and Y be two sequences over alphabet Σ (for DNA sequences, $\Sigma = \{A, C, T, G\}$). An *alignment* of X and Y is two sequences X' and Y' over the alphabet $\Sigma \cup \{-\}$, where X' is formed from X by adding only dashes to it, and Y' is formed from Y by adding only dashes to it, such that

- 1 $|X'| = |Y'|$ *i.e.*, X' and Y' have the same size,
- 2 there does not exist an i such that $X'[i] = Y'[i] = -$

This alignment is also referred to as *global pairwise alignment* (as opposed to *local pairwise alignment*, which is used to align selected regions of sequences X and Y).

Sequence alignment helps biologists make inferences about the evolutionary relationship between two DNA sequences. Aligning two sequences amounts to “reverse engineering” the evolutionary process that acted upon the two sequences and modified them so that their characters and their lengths differ. As an example, one possible alignment of the two sequences $X = ACCT$ and $Y = TACGGT$ is as follows:

$$\begin{array}{rcccccccc} X' & = & - & A & C & - & C & T \\ Y' & = & T & A & C & G & G & T \end{array}$$

As you may imagine, there may be multiple alignments for the same pair of sequences. For example, a trivial alternate alignment for X and Y is as follows:

$$\begin{array}{rcccccccccccc} X'' & = & A & C & C & T & - & - & - & - & - & - \\ Y'' & = & - & - & - & - & T & A & C & G & G & T \end{array}$$

2.2 Scoring in Pairwise Sequence Alignment: Optimality Criterion

As discussed above, a number of alignments exist for a given pair of sequences; therefore, we define a *scoring scheme* that gives higher scores to “better” alignments. Once the scoring scheme is defined, we seek an alignment with the highest score (among all feasible alignments). For DNA, a scoring scheme is given by a 5×5 matrix M , where for $p, q \in \{A, C, T, G\}$, $M_{p,q}$ specifies the score for aligning p in sequence X' with q in sequence Y' , $M_{p,-}$ denotes the penalty for aligning p in sequence X' with a dash in sequence Y' , and $M_{-,q}$ denotes the penalty for aligning q in sequence Y' with a dash in sequence X' . Assuming $|X'| = |Y'| = k$, the score of the alignment is

$$\sum_{i=1}^k M_{X'[i], Y'[i]}. \tag{1}$$

For this assignment, we will assume the following scoring scheme: $M_{p,p} = 5$, $M_{p,q} = 2$ (for $p \neq q$), $M_{p,-} = -2$ and $M_{-,q} = -4$.

For this scoring scheme, the score of the (X', Y') alignment in Section 2.1 is

$$M_{-,T} + M_{A,A} + M_{C,C} + M_{-,G} + M_{C,G} + M_{T,T} = (-4) + 5 + 5 + (-4) + 2 + 5 = 9$$

and the score of the (X'', Y'') alignment is $4 \times M_{p,-} + 6 \times M_{-,q} = -32$.

2.3 Sequential Algorithm to compute the Optimal Scoring for Pairwise Sequence Alignment

In this problem, we introduce a sequential dynamic programming algorithm (called the Smith-Waterman algorithm) to compute the Optimal Scoring for Pairwise Sequence Alignment. For two sequences X and Y of lengths m and n , respectively, denote by $S[i, j]$, $0 \leq i \leq m$ and $0 \leq j \leq n$, the score of the best alignment of the first i characters of X with the first j characters of Y . The boundary values are, $S[i, 0] = i * M_{p,-}$ and $S[0, j] = j * M_{-,p}$. It has been shown that this optimal scoring can be defined as follows $\forall i, j \geq 1$:

$$S[i, j] = \max \begin{cases} S[i-1, j-1] + M_{X[i],Y[j]} \\ S[i-1, j] + M_{X[i],-} \\ S[i, j-1] + M_{-,Y[j]} \end{cases} . \quad (2)$$

The above definition directly leads to a sequential dynamic programming algorithm that can be implemented as shown in Listing 1. Assume that the input sequences are represented as Java strings, and the scoring matrix, S , is represented as a 2-dimensional array of size $(X.length()+1) \times (Y.length()+1)$. After the algorithm terminates, the final score is available in $S[X.length()][Y.length()]$.

The dependence structure of the iterations in Listing 1 is shown in Figure 1. The cells in the figure correspond to $S[i, j]$ values, and the arrows show the dependences among the $S[i, j]$ computations.

```

1  for ( i = 1; i <= xLength; i++)
2    for ( j = 1; j <= yLength; i++) {
3      int i = point.get(0);
4      int j = point.get(1);
5      char xChar = X.charAt(i-1);
6      char YChar = Y.charAt(j-1);
7      int diagScore = S[i-1][j-1] + M[charMap(xChar)][charMap(YChar)];
8      int topColScore = S[i-1][j] + M[charMap(xChar)][0];
9      int leftRowScore = S[i][j-1] + M[0][charMap(YChar)];
10     S[i][j] = Math.max(diagScore, Math.max(leftRowScore, topColScore));
11   }
12   int finalScore = S[xLength][yLength];

```

Listing 1: Sequential implementation of Smith-Waterman Algorithm for Optimal Scoring for Pairwise Sequence Alignment

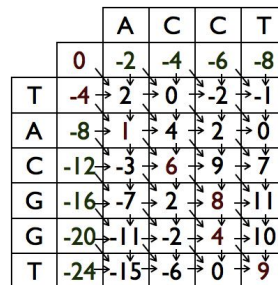


Figure 1: Dependences in Pairwise Sequence Alignment

This homework focuses on computing the optimal score for pairwise sequence alignment, not on the alignment itself. Though a biologist is ultimately interested in seeing the alignment, there are many applications where the score alone is of interest. For example, in multiple sequence alignment, the most commonly used approach is called progressive alignment, where an evolutionary tree is first built based on the scores of pairwise alignments, and then the tree is used as a guide for doing the multiple sequence alignment. In this case, the pairwise alignments are performed solely for the sake of obtaining scores, and the alignments

themselves are not needed. However, it is important to compute the scores as quickly as possible when exploring alignments of large DNA sequences.

2.4 Your Assignment: Parallel Optimal Scoring for Pairwise Sequence Alignment

Your assignment is to design and implement parallel algorithms for optimal scoring for pairwise sequence alignment. We have provided a sequential implementation of the algorithm in `SeqScoring.java` that you can use as a starting point. You should not use phasers for checkpoint 1. You should not use any parallel data constructs inside a constructor. Your homework deliverables are as follows:

1. **[Checkpoint 1 due on March 22, 2021: Ideal parallelism with abstract execution metrics (20 points)]** Examine the dependence structure for $S[i, j]$ defined in Section 2.3 and create an ideal parallel version called `IdealParScoring.java` that computes the same output as `SeqScoring.java`, and delivers the maximum ideal parallelism ignoring all overheads. For analysis of ideal parallelism, assume that computing a single element of $S[i, j]$ takes one unit of time, *e.g.*, by inserting a call to `doWork(1)` between lines 9 and 10 of Listing 1. You will need to insert this `doWork()` call at the appropriate location in the parallel solution you create in `IdealParScoring`. Your solution will be evaluated using HJlib's abstract metrics. The abstract metric costs used will be those from Homework 1, *i.e.* they will not include the `async spawn` cost from Homework 2. You should not use phasers for Checkpoint 1. You may use phasers after Checkpoint 1.

For this checkpoint, we have some unit tests in `Homework3Checkpoint1CorrectnessTest.java`.

Hints based on common errors/omissions from past years: Remember to check that your solution passes all unit tests, and that you don't have any checkstyle errors.

2. **[Final submission due on April 5, 2021: Useful parallelism on NOTS compute nodes (40 points)]** Create a new parallel version of `SeqScoring.java` that is designed to achieve the smallest execution time using 16 cores on a dedicated NOTS compute node. Note that this is real execution time, not abstract metrics. Your code for this part will need to go into the `UsefulParScoring.java` file.

For this part of the assignment, we recommend first debugging your solution on small strings for correctness (which can be done on any platform) using `Homework3Checkpoint2CorrectnessTest`, and then evaluating the performance of your implementation with pairs of strings of length $O(10^4)$ on dedicated NOTS compute nodes using `Homework3PerformanceTest`. Lab 5 will provide instructions on submitting jobs to the NOTS cluster.

Even though each NOTS compute node has 32GB (or more) of memory, we will evaluate all homeworks using a maximum heap size of 8GB. The JVM heap size for tests running on NOTS is set in the provided `pom.xml`. Your submission will be evaluated with 8GB of heap, so changing this value in your `pom.xml` may result in incorrect test results. If you are running the JUnit tests locally through IntelliJ rather than using the provided `pom.xml`, you will want to add the following JVM command line argument to your Run Configurations to ensure that the JVM launched by IntelliJ is allowed to allocate up to 8GB of memory (in addition to the `-javaagent` argument that should already be there): `-Xmx8192m`

However, note that most laptops do not have 8GB of physical memory, so running some of the larger tests locally may be prohibitively slow as your machine swaps memory pages out to disk as you exceed physical memory capacity.

For this checkpoint, we have provided a set of unit tests in `Homework3Checkpoint2CorrectnessTest.java`. The `testUsefulParScoring` and `testUsefulParScoring2` tests in `Homework3PerformanceTest.java` also evaluate the performance of your `UsefulParScoring` implementation against the sequential version. We have provided a SLURM file under `src/main/resources` that can be used on NOTS to submit `Homework3PerformanceTest` for testing on a compute node. Note that you will need to edit this SLURM file to supply your e-mail for notification and to provide the correct path to your `hw_3` folder on NOTS.

Hints based on common errors/omissions from past years: Remember to check that your solution passes all unit tests, and that you don't have any checkstyle errors. Also, you should aim to get a speedup of $\geq 10\times$ for this part; you will get a 1-point deduction if the speedup is in the $[9, 10)$ range, a 2-point deduction if it is in the $[8, 9)$ range, etc.

3. **[Homework report (15 points)]** With the final submission you should submit a report file, formatted as a PDF file named `hw3_report.pdf`, summarizing the design of your parallel algorithms in `IdealParScoring.java` and `UsefulParScoring.java`, explaining why you believe that each implementation is correct and data-race-free. Your report should also include the following measurements for `UsefulParScoring.java` Execution time of `SeqScoring.java` and `UsefulParScoring.java` on a NOTS compute node with inputs of length 10,000. You can get these numbers from a run of the `Homework3PerformanceTest.testUsefulParScoring` test on NOTS (manually).