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TL;DR

Want a quick overview of what to do with no details? http://bit.ly/201spring19-dna-tldr

Project Introduction

BackGround

This background is interesting, but not really needed to do the assignment. There are some good stories here, but if you want to get to the assignment, you can skip this stuff.

In this assignment you'll experiment with different implementations of a simulated <u>restriction</u> <u>enzyme</u> cutting (or cleaving) a DNA molecule. <u>Three scientists shared the Nobel Prize</u> in 1978 for the discovery of restriction enzymes. They're also an essential part of the process called <u>PCR polymerase chain reaction</u> which is one of the most significant discoveries/inventions in chemistry and for which Kary Mullis won the Nobel Prize in 1993.

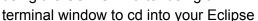
Kary Mullis, the inventor of PCR, is an interesting character. To see more about him see this archived copy of a 1992 <u>interview in Omni Magazine</u> or his <u>personal website</u> which includes information about his autobiography *Dancing Naked in the Mind Field*, though you can read this free <u>Nobel autobiography</u> as well.

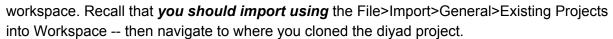
The simulation is a simplification of the chemical process, but provides an example of the utility of linked lists in implementing a data structure. The linked list code you'll write and reason about is an example of a chunk list.

Git

Fork, clone, and import the cloned project from the file system. Use this URL from the course GitLab site: https://coursework.cs.duke.edu/201spring19/dna-link-spring19 . Be sure to fork first (see screen shot). Then Clone

using the SSH URL after using a





△ ∨ ☆ Star 1 🦞 Fork 107

DO NOT DO NOT import using the Git open -- use General>Existing Projects Into Workspace.

Pushing to Git

When you make a series of changes you want to 'save', you'll push those changes to your GitHub repository. You should do this after major changes, certainly every hour or so of coding. You'll need to use the standard Git sequence to commit and push to GitHub:

git add .

```
git commit -m 'a short description of your commit here'
git push
```

Partners

You may work with a partner *from your discussion section* on this assignment. One person should fork-and-clone from the GitLab repo. That person will add the other person/partner as a collaborator on the project. For full information, see the documentation here: https://docs.gitlab.com/ee/user/project/members/

Choose Settings>Members>Invite Members. Then use the autocomplete feature to invite your partner to the project. Both of you can clone and push to this project.

- 1. First, one person should create the GitLab repository then add the partner as a maintainer to the project.
- 2. Both students should clone the same repository and import it into Eclipse.
- 3. After both students have cloned and imported, one person should add a comment to the LinkStrand.java class with their name in a comment at the start of the file. Commit and push this change.
- 4. The other partner will then use the command line and issue a git pull request. Simply use the command-line and type:

git pull

5. After this command, right-click on the project in Eclipse and choose the Refresh menu item. You should see the modified LinkStrand.java file with a new comment. Add your name in a comment, then commit and push. The other person will need to issue a git pull to get that file.

As long as partners are modifying different files, this process works seamlessly. Modifying the same file can lead to issues in resolving conflicts. Git will deal with this with your help, but it's better to take turns in working on the same file, or to work on different files within the project. *Ideally you'll always be physically together when working on the project.*When submitting you'll use the partner/team in Gradescope. That's described below in the submission section.

Can't find partner in discussion? Request a partner: http://bit.ly/201spring19-dna-partnerrequest

Overview of Programming

You'll run benchmarks for three classes, StringStrand, StringBuilderStrand and LinkStrand. They are different implementations of the IDnaStrand Interface. The first two are provided in the starter code and you'll complete the implementation of the class

LinkStrand. You'll also design, develop, and run benchmark classes as part of the analysis section.

This assignment has two parts: <u>Part 1 (due before Spring Break)</u> consists of cloning the starter repo and answering Questions 1 and 2 of the analysis only: No code is required for this part. <u>Part 2 (due after Spring Break)</u> consists of writing the code for the LinkStrand and CodonProfiler classes, and then answering Question 3 of the analysis.

There are four components to this assignment:

- [Part 1] Run benchmarks on two provided classes. Describe the results of running the benchmarks in your <u>analysis.txt</u> file. The description of what to do for running the benchmarks is described in the <u>Benchmark Results section</u>. You can run two of the three benchmarks before completing the implementation of <u>LinkStrand</u> described next. Complete this before Spring break, no programming.
- 2. **[Part 2]** Implement LinkStrand that extends the IDnaStrand interface so that it is correct and meets performance requirements. Test and benchmark this class and report on these tests in your analysis.txt file.
- 3. [Part 2] Change the implementation of CodonProfiler.getCodonProfile so that it runs in O(N) time instead of O(C×N) time for an array of C codons and a strand of N characters.
- 4. **[Part 2]** Answer questions about the benchmark code. See the <u>Analysis section</u> for details.

LinkStrand implements IDnaStrand

Create a new class named LinkStrand. This class must implement the IDnaStrand interface as explained in some detail below. You should allow Eclipse to fill in all the methods needed to implement the interface with stub interfaces, e.g., that return null or zero for example. Then you'll implement and test the methods as described here and in the section that follows on how the class works. Here's the header for the class that you'll implement:

public class LinkStrand implements IDnaStrand

If you let Eclipse add the unimplemented methods you'll see @Override with seven methods that are described below.

You'll implement two constructors as described below. The constructors and methods don't need to be implemented in the order shown, but the simpler methods are listed first. These methods are tested in the **TestStrand** class except for **charAt** which is tested in the **TestIterator** class. In descriptions below **n** is the number of nucleotides/basepairs/characters in a strand.

- 1. Implement two constructors: **one with no parameters (the default constructor)** and one with a **String** parameter.
 - a. The constructors work by calling the required initialize method, see StringStrand for an example.
- 2. Implement the initialize method that initializes the LinkStrand object with a String.
- 3. Implement the getInstance method that works similarly to what you see in StringStrand and StringBuilder strand. This must return a LinkStrand object.
- 4. Implement size. This should be a single line and must run in O(1) time.
- 5. Implement getAppendCount. This should be a single line and must run in O(1) time.
- 6. Implement toString. This returns the String representation of the LinkStrand by looping over nodes and appending their values to a StringBuilder object. The method should run in O(N) time.
- 7. Implement append which creates one new node and updates instance variables to maintain class invariants as described below.
- 8. Implement reverse to return a new LinkStrand object that's the reverse of the object on which it's called. *This method is not a mutator, it creates a new LinkStrand.*
- 9. Implement charAt which returns the character at a specific index. This method requires new instance variables to meet performance characteristics.

You should test each method as you implement it using the TestStrand JUnit test class. You'll need to change the type of strand returned in that JUnit class method getNewStrand to test your class. It's unlikely that any tests will work until you've implemented

LinkStrand.toString().

LinkStrand State, Constructors and initialize method

You should start with the following definitions for a private inner class and instance variables to use a linked-list internally as part of the LinkStrand class. **Note that all are private**.

```
private class Node {
   String info;
   Node next;
   public Node(String s) {
        info = s;
        next = null;
   }
}
private Node myFirst,myLast;
private long mySize;
```

private int myAppends;

All constructors and methods must maintain the following class invariants:

- 1. myFirst references the first node in a linked list of nodes.
- 2. myLast references the last node in a linked list of nodes.
- 3. mySize represents the total number of *characters* stored in all nodes together.
- 4. myAppends is the number of times that the append method has been called. It would be useful to think of this as one less than the number of nodes in the linked list.

info

Initially, when the LinkStrand("cgatt") constructor is called (though the String parameter can be any string) there will be a single Node in the linked list that represents the DNA strand "cgatt". (The only way to have more than one node in a LinkStrand internal linked-list is by calling .append.)

As described above, you'll create two constructors. The string constructor should consist of **one call to** initialize which establishes the class invariant with a single node representing the entire strand of DNA as illustrated above. The no-argument constructor, sometimes called the default constructor, should have one line: this("") which calls the other constructor with a string parameter of "".

The initialize method will maintain the class invariants when it's called. There will be a single node created after initialize is called.

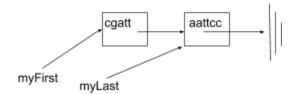
Implementing the append Method

The append method should add one new node to the end of the internal linked list and update state to maintain the invariant.

For example, suppose that these two statements are both executed:

```
LinkStrand dna = new LinkStrand("cgatt");
dna.append("aattcc");
```

The internal linked list maintained by **LinkStrand** after the first call is diagrammed above. After the call to append we have the following picture:



Note that maintaining the class invariant after this call to append would require

- 1. myFirst doesn't change
- 2. myLast changes to point to the new node added
- 3. mySize is incremented by six
- 4. myAppends is incremented by one (because a new node is added).

Note that .append returns an IDnaStrand object. This is the object that was just modified/appended to. However, the method append *does not* create a new IDnaStrand object. The .append method is a mutator -- it changes the internal state of the IDnaStrand object on which it's invoked, and then returns this LinkStrand object itself. Look carefully at both StringStrand and StringBuilderStand strand to see what to return.

Note that after implementing append, the method getAppendCount should return the correct result, the value of instance variable myAppends that's maintained by the class invariants and initialized/updated in initialize and append.

Implementing the toString method

The toString method returns the String representation of the entire DNA strand.

Conceptually this is a concatenation of the String stored in each node.

This method should use a standard while loop to visit each node in the internal linked list. The method creates and updates a single StringBuilder object by appending each node.info field to a StringBuilder object that's initially empty. The final return from LinkStrand.toString will simply be returning the result of calling .toString() on the StringBuilder object. See the DNABenchmark.dnaFromScanner implementation for guidance on the StringBuilder strand class.

For more guidance on StringBuilder, see the Java Documentation here.

You should be able to test all the methods implemented to this point using the class <code>TestStrand</code>. The testing methods in <code>TestStrand</code> rely on <code>.toString</code> being correct, so after implementing <code>.toString</code> you may find errors in your other methods as a result of testing.

Implementing the reverse method

This method creates a new LinkStrand object that is the reverse of the object on which it's called. The reverse of "cgatccgg" is "ggcctagc". This method returns a new strand; it does not alter the strand on which it's called, i.e., it's not a mutator.

Note: you must create N new nodes in reversing a LinkStrand object with N nodes. If you do not, you are likely mutating/changing the LinkStrand being reversed.

You'll need to reverse the linked list, and reverse each string in each node of the linked list.

Specifically, the reversed LinkStrand should have the same number of nodes as the original LinkStrand, but in reverse order; each internal node should also contain the reversed String of the corresponding node in the original LinkStrand.

To reverse a String use a StringBuilder appropriately --- see StringStrand.reverse for details on using the StringBuilder.reverse method.

Note that in creating a new linked list that's the reverse of the list of nodes being traversed it's easiest to simply add a new node to the front of the reversed list being constructed. So in reversing a->b->c->d and traversing in order a,b,c,d, your code would have created the list c->b->a after traversing the first three nodes: a,b,c. When reaching the next or 'd' node your code adds 'd' to the front of this list creating d->c->b->a.

Implementing the charAt method

This method returns the character at the specified index if that's a valid index, and throws an IndexOutOfBoundsException otherwise. A naive implementation of this method would start at the beginning of the linked list, the node referenced by myFirst and count characters until the index-th character is found.

For full credit (and to pass the timing tests in TestIterator) you'll need to maintain state so that after a call of charAt(k) the call of charAt(k+1) is an O(1) operation. This will make the loop below O(N) for an N-character strand. See the next section for help on this.

Basic, Correct but Inefficient Implementation of charAt

First we'll show an inefficient implementation of the charAt method --- a method to find a character at a specific index in a linked list of strings. Your code will need to traverse the linked list counting characters. The code below illustrates how to do this. It doesn't check to see if parameter index is valid, but it passes the JUnit tests for correctness.

```
public int charAt(int index) {
   int count = 0;
```

```
int dex = 0;
Node list = myFirst;
while (count != index) {
    count++;
    dex++;
    if (dex >= list.info.length()) {
        dex = 0;
        list = list.next;
    }
}
return list.info.charAt(dex);
}
```

This code will pass correctness tests, e.g., in **TestIterator**. However, it's not efficient since it starts at the beginning of the linked list for each call.

You should be sure you understand how local variables count and dex are used in the code above before trying to make the code more efficient for a sequence of calls as explained in the next section.

Efficient Implementation of charAt

You should create instance variables in the class LinkStrand so that after a call of charAt(k), calling charAt(k+1) is an O(1) operation.

You can see in the code above that three values are used, these correspond to the three variables shown above:

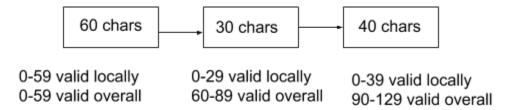
- the current node in the iteration (list),
- the current index in that node (dex),
- the overall count (count).

You should *create and initialize three corresponding instance variables*: one for the current node in a sequence of calls of <code>charAt</code>, one for the current index into that node, and one for the overall count. You'll need to initialize these instance variables when a strand is created, e.g., in method <code>initialize</code>. You'll use these instance variables on each call to <code>charAt</code>, and you'll update them similarly to how the local variables are updated -- to save the current "progress" so that on a subsequent call to <code>charAt</code> it might be possible to continue from the last call and access the next character in a node, for example, by simply incrementing the index into that node. Of course this might require going to the next node if the current node is "out" of characters just as is done in the code shown above.

Use these three instance variables and update them appropriately in charAt:

• myIndex is the value of the parameter in the last call to charAt. This means that if a call to s.charAt(100) is followed by s.charAt(101) the value of myIndex will be 100 after s.charAt(100) executes and 101 after s.charAt(101) executes.

• myLocalIndex is the value of the index within the string stored in the node last-referenced by charAt when the method finishes. For example, suppose a strand consists of three nodes: the first has 60 characters; followed by a node of 30 characters; followed by a node of 40 characters. The call s.charAt(40) will mean that myIndex is 40 and myLocalIndex is also 40 since that's the index within the first node of the list,



where the character whose index is 40 is found. Suppose this is followed by s.charAt(70). The character at index 60 of the entire strand will be the character with index zero of the second node -- since the first node holds characters with indexes 0-59 since its info field is a string of 60 characters. The character at index 70 of the entire strand will be the character with index 10 of the second node.

myCurrent is the node of the internal list referenced in the last call to charAt. In the example above the value of myCurrent would be the first node after the call s.charAt(40), would be the second node after the call s.charAt(70) or s.charAt(89), and would be the third node after the call s.charAt(90) since the first two nodes only contain a total of 90 characters, with indexes 0 to 89.

In the TestIterator code you get with this assignment, there are correctness tests and performance tests for going forward in O (N) time as described here.

Why do we need **charAt** to be efficient?

If the charAt method is not efficient, the loop below will be $O(N^2)$ since the charAt method will be O(k) to access the k^{th} character.

```
LinkStrand dna = new LinkStrand("....");
StringBuilder s = new StringBuilder("");
for(int k=0; k < dna.size(); k++) {
    s.append(dna.charAt(k));
}</pre>
```

This charAt method is called by the code in the CharDnaIterator class. So iterating over an IDnaStrand object will ultimately use the charAt method as shown in the code below.

```
LinkStrand dna = new LinkStrand("....");
Iterator<Character> iter= dna.iterator();
for(char ch : iter) {
    System.out.print(ch);
```

```
}
System.out.println();
```

The Iterator object in the code above is constructed as a result of calling the default IDnaStrand.iterator method, the body is shown here:

```
return new CharDnaIterator(this);
```

Note that the IDnaStrand object referenced by this is then stored in the CharDnaIterator object being created.

You only need to implement charAt, then all the code described and shown above will work correctly! You will need to initialize the instance variables too.

Order of Calls Matters

However, you'll need to write code to deal with calls that aren't "in order". If the call .charAt(100) is followed by the call .charAt(30) you'll need to start at the beginning of the internal linked list to find the character with index 30. If .charAt(100) is followed by .charAt(350) you won't start at the first node, but continue with the values stored in the instance variables.

CodonProfiler

The class you're given has a method that determines how many times each 3-character codon in an array of codons occurs in a strand of DNA. You should look at the implementation of <code>getCodonProfile</code> and the tests in <code>CodonProfileTest</code> that run the code to see what's expected. The code you're given runs in <code>O(C × N)</code> time for an array of <code>C</code> codons and a stand of <code>N</code> characters. Verify this by looking at the code. The outer loop goes every each codon, and for each one the entire strand is searched via an iterator to find how many times that codon occurs.

Replace this implementation using a HashMap so that the code runs in O(N) time.

You should count how many time every possible codon in the strand occurs using the map. After looking at every possible codon in the strand, and counting each one regardless of whether it is in the array codons, write code to loop over the values codons to create the array to return. Technically this will be O(N+C) since you must loop over all the codons after creating the map.

Benchmark Results

You'll need to run the **DNABenchmark** class three times, once for each implementation of the IDnaStrand interface: **StringStrand**, **StringBuilderStrand**, and **LinkStrand**. You

change the runs by changing the value of the static instance variable strandType at the top of the class file. You should copy/paste the output that's generated by running the benchmark program using the large ecoli.txt file that's in the data folder you get when the project is cloned. The benchmark runs until memory is exhausted. Results are shown from an instructor/TA laptop. You should generate your own results from the machine you run the benchmark code on. The StringStrand class will take a very long time to run!

Your results will not be the same as those shown here, and you may run out of memory with more or fewer experiments. But you should copy/paste the results of your runs into your analysis.txt file and explain the results (see the <u>Analysis section</u> for details).

Note that the benchmark code runs two experiments to average the results. So the time for **StringStrand** in real time is much longer than what's reported as the average (at least double, then more).

Benchmark for StringStrand

These results take a long time to run before exhausting memory. **Anticipate more than 15 minutes.** Generated running **DNABenchmark** with **strandType** to "StringStrand"

dna length = 4,639,221
cutting at enzyme gaattc

Class	splicee	recomb	time appe	nds
StringStrand:	256	4,800,471	0.421 1290	
StringStrand:	512	4,965,591	0.394 1290	
StringStrand:	1,024	5,295,831	0.420 1290	
StringStrand:	2,048	5,956,311	0.479 1290	
StringStrand:	4,096	7,277,271	0.587 1290	
StringStrand:	8,192	9,919,191	0.822 1290	
StringStrand:	16,384	15,203,031	1.290 1290	
StringStrand:	32,768	25,770,711	2.207 1290	
StringStrand:	65,536	46,906,071	4.455 1290	
StringStrand:	131,072	89,176,791	9.741 1290	
StringStrand:	262,144	173,718,231	22.162	1290
StringStrand:	524,288	342,801,111	44.144	1290
StringStrand:	1,048,576	680,966,871	82.143	1290

Exception in thread "main" java.lang.OutOfMemoryError: Java heap space

at StringStrand.append(StringStrand.java:70)

at IDnaStrand.cutAndSplice(IDnaStrand.java:41)

. . .

Benchmark for StringBuilderStrand

Changing strandType to "StringBuilderStrand" yields the results below on an instructor laptop. Memory runs out much more quickly, in seconds, but with the same size as StringStrand.

```
dna length = 4,639,221
cutting at enzyme gaattc
```

Class splicee recomb time appends ____ 256 4,800,471 0.026 1290 StringBuilderStrand: 512 4,965,591 0.020 1290 StringBuilderStrand: StringBuilderStrand: 1,024 5,295,831 0.007 1290 5,956,311 0.006 1290 StringBuilderStrand: 2,048 7,277,271 0.006 1290 StringBuilderStrand: 4,096 9,919,191 0.009 1290 StringBuilderStrand: 8,192 15,203,031 0.010 1290 StringBuilderStrand: 16,384 25,770,711 0.022 1290 StringBuilderStrand: 32,768 46,906,071 0.031 1290 StringBuilderStrand: 65,536 StringBuilderStrand: 131,072 89,176,791 0.069 1290 StringBuilderStrand: 262,144 173,718,231 0.159 1290 StringBuilderStrand: 524,288 342,801,111 0.402 1290

```
Exception in thread "main" java.lang.OutOfMemoryError: Java heap space
    at java.base/java.util.Arrays.copyOf(Arrays.java:3744)
    at
```

1,048,576

680,966,871 0.631 1290

java.base/java.lang.AbstractStringBuilder.ensureCapacityInternal(Abstr actStringBuilder.java:146)

. . .

StringBuilderStrand:

Benchmark for LinkStrand

Generated running **DNABenchmark** with **strandType** to "**LinkStrand**" after that class has been tested. Note that this takes just seconds to run, and strand/splicee sizes are significantly larger than with the other **IDnaStrand** types.

```
dna length = 4,639,221
cutting at enzyme gaattc
----
Class splicee recomb time appends
----
```

LinkStrand:	256	4,800,471	0.028	1290
LinkStrand:	512	4,965,591	0.023	1290
LinkStrand:	1,024	5,295,831	0.005	1290
LinkStrand:	2,048	5,956,311	0.003	1290
LinkStrand:	4,096	7,277,271	0.004	1290
LinkStrand:	8,192	9,919,191	0.006	1290
LinkStrand:	16,384	15,203,031	0.004	1290
LinkStrand:	32,768	25,770,711	0.003	1290
LinkStrand:	65,536	46,906,071	0.004	1290
LinkStrand:	131,072	89,176,791	0.004	1290
LinkStrand:	262,144	173,718,231	0.003	1290
LinkStrand:	524,288	342,801,111	0.004	1290
LinkStrand:	1,048,576	680,966,871	0.006	1290
LinkStrand:	2,097,152	1,357,298,391	0.004	1290
LinkStrand:	4,194,304	2,709,961,431	0.006	1290
LinkStrand:	8,388,608	5,415,287,511	0.003	1290
LinkStrand:	16,777,216	10,825,939,671	0.003	1290
LinkStrand:	33,554,432	21,647,243,991	0.006	1290
LinkStrand:	67,108,864	43,289,852,631	0.005	1290
LinkStrand:	134,217,728	86,575,069,911	0.006	1290
LinkStrand:	268,435,456	173,145,504,471	0.005	1290
LinkStrand:	536,870,912	346,286,373,591	0.004	1290
LinkStrand:	1,073,741,824	692,568,111,831	0.005	1290

Exception in thread "main" java.lang.OutOfMemoryError: Java heap space
 at java.base/java.util.Arrays.copyOf(Arrays.java:3744)

JUnit Tests

You should run the JUnit tests in both TestStrand and TestIterator. Verify that these work for StringStrand and StringBuilderStrand and then use these classes to test your LinkStrand implementation. You'll use the CodonProfilerTest to test the code you write in CodonProfile.

Analysis

Answer three questions in your analysis.txt file. The questions are here: http://bit.ly/201spring19-dna-analysis -- The document includes detailed explanations and diagrams, be sure to read that and to not only rely on on what's in analysis.txt.

For DNA Part 1, due before Spring Break, you'll only submit the answers to the first two analysis questions on StringStrand and StringBuilderStrand classes. You'll push your project to Git and then Gradescope, but only the analysis.txt file will be looked at by the UTAs. You do not need to write any code for this part.

For DNA Part 2, due after Spring Break, you'll write the code for LinkStrand and answer the third question.

After completing the analysis questions you should push to Git and submit the entire project on Gradescope. Please note that Analysis is part of the assignment, and Gradescope is the only portal to submit the assignment, including the analysis. We reserve the right to reject your analysis submission if you forget to upload it to Gradescope, even if it's in your Git repo.

Submitting

You'll submit the code to Gradescope after pushing your program and analysis.txt file to GitLab. This is a partner/team project in Gradescope, so one person will be able to add the other as partner if you're working together. *Only one person a group submits, not both.*

Refer to this document for submitting to Gradescope with a partner:

Reflect

You can access the reflect form at http://bit.ly/201spring19-dna-reflect

You should NOT complete the reflect form until you're done with all the coding portion of the assignment. Since you may uncover bugs from the autograder, you should wait until you've completed debugging and coding before completing the reflect form.

Grading

Points	Grading Criteria
16	Code for LinkStrand. This includes 4 for correct and efficient implementation of .charAt method, as well as 2 for API <i>and</i> Javadoc comments in LinkStrand.
4	Implementation of CodonProfiler that runs in O(N) time and is correct.
8	Analysis code and questions answered. UTAs will grade and comment on this. Part 1 is 6 points, part 2 is 2.

2 Comments and code style. UTAs will grade and comment on this.

See this piazza post for expectations of Javadoc comments. After writing the comments you should push to Git and submit the entire project on Gradescope.

We will map total points you earn to scores as follows. This means if you lose five points, you receive the same score as losing zero points: an A.

25-30: A 19-24: B 13-18: C 8-12: D