EteRNA University - How to Build a Bot 26 Feb, 2014

Teacher: Jnicol

Boiled down lesson - Work in progress (Raw original chat can be found here)

Hi everyone, Welcome to EteRNA Class Time!

In this class we will learn how to Build A Bot. A bot, in EteRNA, is a computer program that will automatically solve a puzzle. We want to pass the dot-bracket structure to the bot and expect an RNA sequence to be returned that will correctly fold into this structure.

For instance, if we pass the structure (((....))) to the bot, we would expect a sequence like **CCCAAAGGG** to be returned. Since this is an interactive class, lets open some windows you will need to participate.

Open the scripting interface window where the bot's code will be written,

http://eterna.cmu.edu/web/script/create/

I would like to use firedrake's suggestion and have the class try to work out the code for each task, and if needed, I will help out after a few minutes. The first task is to use the scripting interface window to input a structure (in the input box) and have that same structure string returned in the Result console.

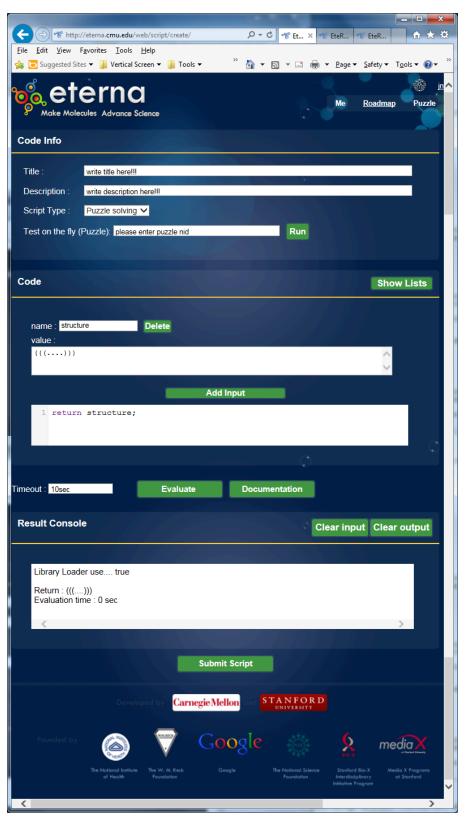
inicol: did anyone create an input box and display the structure?

firedrake969: How do I read the input? jnicol: when you name the input box

jnicol: use the same name in your program

firedrake969: So var input = [what?]

This is what the code window should look like,



http://amelior.com/eterna/classtime/Class3 Task1.png

Here is how to do it. Click add input.



This will give you some fields where you can start making a program.

Code		Show Lists
nama :	Delete	
name : name value :	Delete	
value		.:
	Add Input	
1		

Big or small letter matters. If you write return sequence with big R, it will not become activated.

firedrake969: outln(structure);

inicol: thats all you need for now!

jnicol: the return value will be read when we run test puzzles against the script

jnicol: so thats why we don't want to just use outln. Now, instead of returning the structure, lets return a sequence. For the second task, replace all (with a C, all) with a G and all . with an A. Javascript has a function, replace to make this task easier.

Using **structure.replace**('(', 'C'); will replace the first (with C

Using structure.replace(/[(]/g, 'C'); will replace all occurrences of (with C

Homework

An exercise after this class is to look up the javascript function replace to understand the syntax better.

The Script Documentation List says:
Lib.replace(sequence, index, target)
return sequence which character at index in sequence replaced to target
ex) Lib.replace("AGCU", 2, "A") = "AGAU";

firedrake969: How does the second replace thing work? It seems the same as the first besides

the /[(]/g

firedrake969: instead of just "("

jnicol: every occurrence of "(" will be replaced

firedrake969: And the second one?

inicol: for the second

inicol: the first one will just replace the first occurrence of "("

firedrake 969: Why does it have /g at the end?

inicol: g means global

jnicol: Since () and . are special characters in javascript, a way to escape them is by enclosing

them in []

firedrake969: And how do I get the letter of a a string knowing its position within a string? jnicol:

structure[0]

firedrake969: WHen I put /[(]/g into the first arg of replace(), it turns red, like there's an error

inicol: are you using outln or return?

firedrake969: return

firedrake969: structure.replace(/[(]/g, "C");structure.replace(/[.]/g, "A");structure.replace(/[)]/g,

"G");return structure;

inicol: very nice!

firedrake969: It gives me the original structure though

jnicol: I came up with code similar, return structure.replace(/[(]/g, 'C').replace(/[)]/g,

'G').replace(/[.]/g, 'A');

firedrake969: For some reason, mine won't work

jnicol: structure doesn't change, only what is returned from the replace call

firedrake969: So should I give it a new variable that can change?

firedrake969: var newStruct = structure;newStruct.replace(/[(]/g, "C");newStruct.replace(/[.]/g,

"A");newStruct.replace(/[)]/g, "G");return newStruct;

jnicol: you would need to do something like sequence=structure.replace(...

firedrake969: Still returns the original structure

inicol: then return sequence;

firedrake969: var sequence = structure; sequence.replace(/[(]/g, "C"); sequence.replace(/[.]/g,

"A");sequence.replace(/[)]/g, "G");return sequence;

firedrake969: Still gives the original structure

inicol: newstruct=structure.replace(/[(]/g,'C'); return newstruct;

firedrake969: Oddly, that works.

firedrake969: OH ok thanks

firedrake969: I know inicol: not oddly:)

firedrake969: I figured out what happened

jnicol: you need to assign the return value from the replace to a variable

firedrake969: var sequence = structure; sequence = sequence.replace(/[(]/g, "C"); sequence =

sequence.replace(/[.]/g, "A");sequence = sequence.replace(/[)]/g, "G");return sequence;

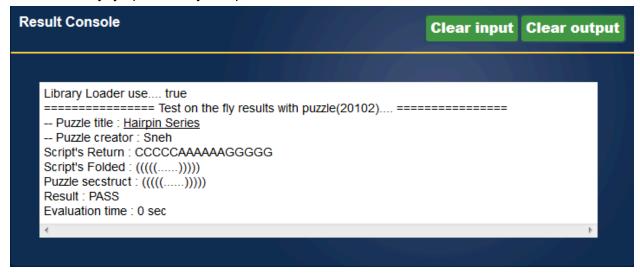


jnicol: ok, good

firedrake969: I just didn't reset it

jnicol: yes

firedrake969: yay I passed my first puzzle



firedrake969: I did Test on the fly with ID 20102

Code Info		0
Title :	write title here!!!	
Description :	write description here!!!	
Script Type :	Puzzle solving ▼	
lest on the lly	(Puzzle): 20102 Run	

jnicol: so you get CCCAAAAGGG as a return?

Re	sult Console	Clear input	Clear outpu
	Library Loader use true		
	Return : CCCAAAAGGG Evaluation time : 0 sec		
	←		F

firedrake969: Yeah

jnicol: Lets take a step back and see what we have.

firedrake969: Well, 5C and 5xG

jnicol: We have input a structure and returned a sequence that we hope will fold into that

structure

firedrake969: Because I had 5x(and 5x)

jnicol: Congratulations, you have just created your first bot!

jnicol: To prove this, we can enter some puzzle ids in Test On The Fly input box and see that our

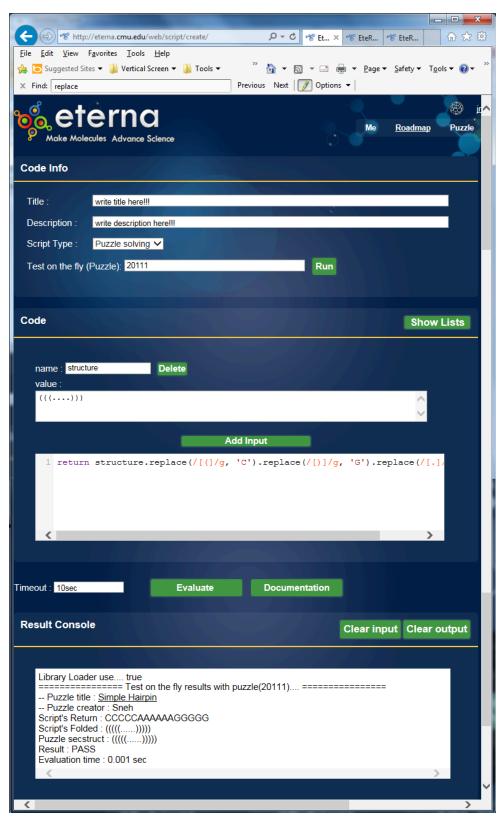
bot can solve them.

jnicol: If we order the challenge puzzles by number of solvers, the first and easiest puzzle is

http://eterna.cmu.edu/web/puzzle/20111/

jnicol: take the puzzle id number, 20111, and put it in the Test on the Fly input box and click run.

jnicol: You should get the following result,



http://amelior.com/eterna/classtime/Class3 Task2.png

jnicol: If we actually Submit Script, we get an additional button, See Results of Player Puzzles, which randomly tests many puzzles. As an example, lets use Meechl's O Christmas Tree script, http://eterna.cmu.edu/web/script/3223005/

Click on the See Results of Player Puzzles, and we see that many puzzles are tested,

http://amelior.com/eterna/classtime/MeechlsScriptResults.png

This script solves 50% of the player puzzles tested and is a great example of how GC pairs can be flipped to solve puzzles. A good exercise would be to read through Meechl's code to see how this was accomplished. The next step for our bot is initialize the sequence with alternating GC/CG pairs. The scripting interface a very useful function for this task, getPairmap.

firedrake969: What does do{for}} do?

firedrake969: i.e. do(condition){for(condition){}}

jnicol: it is a loop to repeat itself when the sequence does not fold properly

Lets see what **getPairmap** can do. Copy this code into the scripting interface window. (Delete previous code)

rnastruc = new RNA(structure);
return rnastruc.getPairmap(structure);

Enter (((....))) in the structure input box and click **Evaluate**

firedrake969: Oh, so you can make a new RNA design an object?

jnicol: there are many functions the devs have provided for the RNA design, yes

firedrake969: Ok, so what does getPairmap() do?

jnicol: You should see this result: Return: 9,8,7,,,,2,1,0 from the code example jnicol: Notice the bases that Puzzlemaker labels as 1-10, javascript labels as 0-9

jnicol: We see from the results that base 0 is paired to base 9, base 1 to 8 and base 2 to 7. Bases 3,4,5,6 do not have pairs. If you open puzzlemaker, it maybe easier to see and grab the structure

http://eterna.cmu.edu/game/puzzlemaker/

firedrake969: I input this

firedrake969: nvm, I see

firedrake 969: But what about the trailing RNA unpaired strand?

inicol: i get

69,68,67,66,65,,64,63,62,61,60,,59,58,57,56,55,,54,53,52,51,50,,49,48,47,46,45,,44,43,42,41,4

0,39,..,35,34,33,32,31,30,28,27,26,25,24,22,21,20,19,18,16,15,14,13,12,10,9,8,7,6,4,3,2,1,0

firedrake969: Same

firedrake969: It's 74 bases long... firedrake969: but it only returns 70

firedrake969: And cuts off the last four bases

inicol: ah, looks like trailing unpaired bases has a bug

inicol: we need to report that to jee

jnicol: I like to use an array to hold the sequence for each base.

inicol: The reason is because if I set sequence = "CCCAAAAGGG";

firedrake969: You can't access it easily or change it

jnicol: I cannot easily update a base, for example I cannot use sequence[3] = 'G'; With an array, I can update each base individually. The following code is an example of how an array can be used to hold and initialize the sequence.

```
rnastruc = new RNA(structure);
pairmap = rnastruc.getPairmap(structure);
sequence = Array();
for (i=0; i<structure.length; i++) {
    sequence[i] = 'A';
}
return sequence.join(");</pre>
```

jnicol: You can use this code as a starting point to generate a sequence with alternating GC pairs. Instead of initializing every base to A, first test the pairmap, then decide if an A, G or C should be used.

firedrake969: rnastruc = new RNA(structure);rnaPairmap = rnastruc.getPairmap(structure);var baseArray = [];for (var i = 0; i < sequence.length; i++) { baseArray[i] = "A";}

firedrake969: Did something slightly different

inicol: I like your initiative!

firedrake969: What's the advantage of using var newArray = Array(); rather than [whatever] = [];

firedrake969: It seems the same, as both set up an empty array

jnicol: not sure, I usually use =Array()

firedrake969: Ok. So it's just a matter of style?

jnicol: yes, coding preference

There is no correct code, only a correct result

Next task is to create a sequence with alternating GC pairs

firedrake 969: For any structure, or explicitly?

inicol: any structure that is input

firedrake 969: So would one approach be to separate the getPairmap into a list somehow?

inicol: correct

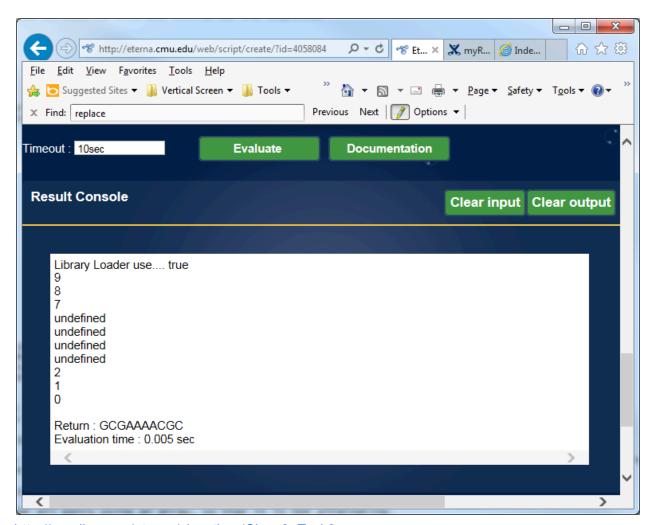
firedrake969: It's kind of hard because it's just ,, rather than , ,

firedrake969: no spaces or anything in between

jnicol: try this

```
rnastruc = new RNA(structure);
pairmap = rnastruc.getPairmap(structure);
sequence = Array();
for (i=0; i<structure.length; i++) {
  outln(pairmap[i]);
}
return sequence.join(");</pre>
```

It shows what the pairmap can be compared to:



http://amelior.com/eterna/classtime/Class3 Task3.png

firedrake969: How does it handle the undefineds and skip the commas? jnicol: commas are not part of the array, they just display when converted to a string

```
jnicol: if (pairmap[i] == undefined) { sequence[i] = 'A'; } for instance firedrake969: Ok and is it undefined or "undefined" (a string)? jnicol: the way the dev programmed getPairmap, it is undefined (without quotes), like null
```

Here is the code I came up with for this task:

```
rnastruc = new RNA(structure);
pairmap = rnastruc.getPairmap(structure);
sequence = Array();
nextbase = 'G';
for (i=0; i<structure.length; i++) {
outln(pairmap[i]);
 if (pairmap[i] == undefined) {
  sequence[i] = 'A';
}
 else if (pairmap[i] > i) {
  sequence[i] = nextbase;
  if (nextbase == 'G') { nextbase = 'C'; }
  else { nextbase = 'G'; }
  sequence[pairmap[i]] = nextbase;
}
return sequence.join(");
```

jnicol: Notice that I put in an **outIn(pairmap[i])**; statement, which is just for debugging purposes. **outIn** is probably the best tool we have for now to find out what is not working as we expect it to.

firedrake969: gives

jnicol: looks good!

firedrake969: Going to implement something that checks if it works

jnicol: this might be a good place to stop, thats the next step for our bot. I actually made a script

that I was hoping to get up to tonight, but it can wait until next week to explain it.

http://eterna.cmu.edu/web/script/4058084/