Bioinformatics-themed projects in Discrete Mathematics

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- My task: Put bioinformatics in Discrete Mathematics course.

Summary of projects

1. Indel; relations: Build insertion-deletion (symmetric) relation from insertion and deletion (anti-symmetric) relations.
2. Sequence alignment (Smith-Waterman); induction (recursive algorithm): Work through examples of a recursive algorithm, and (maybe) prove it works, by induction.
3. Mass spectrometry; counting: If you build a complete database of precise molecular weights of all fragments of strings of molecules, how big would it have to be?
4. Reaction networks (Petri nets); directed graphs: Simulate and analyze dynamical systems from directed graph.
5. Sequence reassembly (SBH); Euler path: Fragments of length b are the edges, and fragments of length $b-1$ are the vertices; then the entire sequence is an Euler trail.
6. Reconstructing phylogenetic trees (UPGMA); rooted trees: Work through examples of an algorithm that re-creates a weighted rooted tree from pairwise distances.

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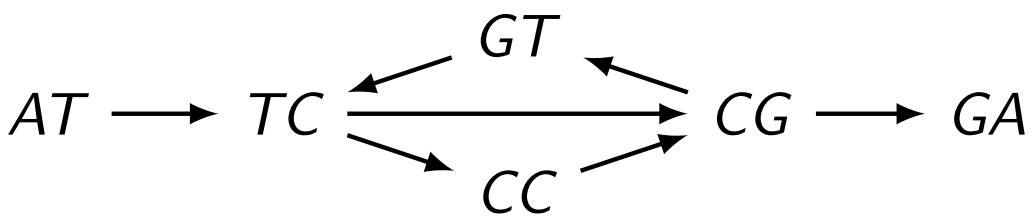

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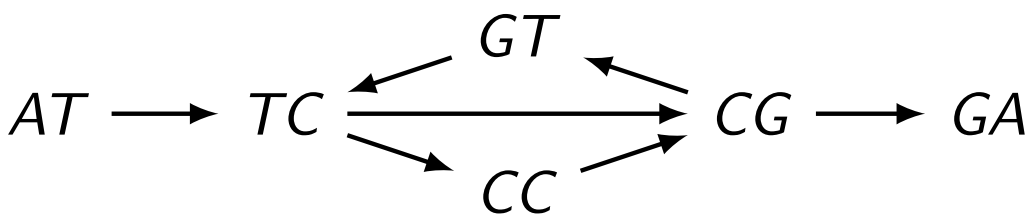

$ATCCGTCGA$ or $ATCGTCCGA$.

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1. Given a string of length 12 (the answer, in some sense). Find the vertices (fragments of length $b - 1 = 2$) and the edges (fragments of length $b = 3$); use these to draw the graph (8 vertices, 10 edges); show how one Euler path reconstructs the string.

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2. Given 10 fragments of length $b = 3$, reconstruct the original string. Parts guide students in parallel to question 1: Find the vertices and the edges; draw the graph (9 vertices, 10 edges); find an Euler path; reconstruct the original string.

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My automation: Program to generate random strings; program to generate all fragments of a string, and a related program to check answers (and help find errors).

How to find topics

One original suggestion was to work in bioinformatics-themed examples when introducing new discrete mathematics topics. This was hard to do, as the students were not familiar with the bioinformatics examples or contexts, so it was not helpful in conveying new discrete mathematics topics. This why I went to projects.

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One difficulty is that, although bioinformatics (especially genomics) is full of algorithms, techniques, and definitions that use discrete mathematics ideas, some of these are more advanced, or don't lend themselves to advancing learning objectives of course.

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- Change some examples every time; others are too hard to change.

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- Students *may* write computer code to solve problem (but not use code written by others), with brief explanation of how they wrote it; not many students have done this, and usually it hasn't been helpful.

Website and acknowledgements

http://www.math.utep.edu/Faculty/duval/class/2300/171/homework.html

(and similar pages for other semesters, since Spring 2010, excluding Fall 2017), to see a semester's worth of projects, including supporting websites and resources.

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