

20.181 Lecture 1

Topics

1. Phylogenetic Inference
2. Molecular Modeling / Protein Design
3. Metabolic Network Modeling & Design

Underlying Relationship

Each Topic has the following components:

1. Data structure
2. Optimization problem
3. Algorithms

Grading

1. HW @ 60%
2. 3 in-class exams at 30% total
3. Class Participation @ 10%

HW Due Dates

HWs are due before midnight 1 week after they are given

Phylogenetic Inference

1. What is phylogenetic inference?
 - Phylogenetic inference is the inference of phylogeny (how's that for a self-referential definition)?
 - Let's try again. Phylogenetic Inference (PI) is the figuring out the family relationship of a set of genetic sequences.
 - [Answers.com](#) weighs in.
 - PI is used to figure out what's what given an otherwise uncharacterized stretch of DNA sequence. For example, if you've just sequenced the genome of a new organism then you would use phylogenetic inference to attempt to figure out what the organism was related to and thus better understand the thing you've just sequenced.
2. Case Studies
 - Young woman in Florida contracted HIV but had no risk factors for it. How to figure out the path by which she had been infected (to warn others and so on). The only small risk factor that she had was that her dentist was

known to be suffering from AIDS. How could you determine the likelihood that the dentist infected his patients with HIV?

- Approach: Note that HIV evolves relatively quickly. For example, on average, HIV genes evolve 1,000,000x faster than human genes. So, do the patients of this dentist have HIV strains that are closer to the dentist's HIV strain than to the rest of the HIV infected population? So, sequence the DNA of HIV collected from patients from the dentist, as well as local residents who also happen to be infected with HIV (as a control group). Then, assemble a family tree to see how the HIV strains of each patient are related to one another. The data suggested that there were a number of patients whose HIV strains were related to the HIV strain of the dentist. Does this mean that the dentist infected his patients? Wikipedia article online [here](#).

3. Phylogenetic Trees (more on this in the next class)

- What do the axes mean?
 - The horizontal axis mean distance. What sort of distance? Time? (no). What then?
 - The vertical axis doesn't mean anything.

4. Quick review of [Recursion](#)

- What is recursion? A function that calls itself over and over again. For example, factorial is a recursive function. $X! = (X)*(X-1)*(X-2)...*(1)$.
- How would we define a recursive function in Python? What are the key attributes? First, a STOP condition. Second, the recursive definition & self-reference. Third, operate on the answer for the self-reference and return the resulting value.
 - Example of a STOP condition. `if (x=0): return 1`
 - Example of self-reference. `return x*(x-1) <-- need to check this.`