CSCE 471/871 Lecture 0: Administrivia

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Welcome to 471/871!

- Check your name on the roster, or write your name if you're not listed
- Policy on sit-ins: You may sit in on the course without registering, but not at the expense of resources needed by registered students
- Introduce yourself
  1. Who are you?
  2. What are you?
  3. Why are you here?
- You should have the following handouts:
  1. Syllabus
  2. Copies of slides

CSCE 471/871 Lecture 1: Introduction

Stephen D. Scott
(With thanks to Andy Benson and Jitender Deogun)

Outline

- What is bioinformatics?
- Relevant biology background
- Fundamental questions in bioinformatics
- What we will (and will not) cover in this course

What is Bioinformatics?

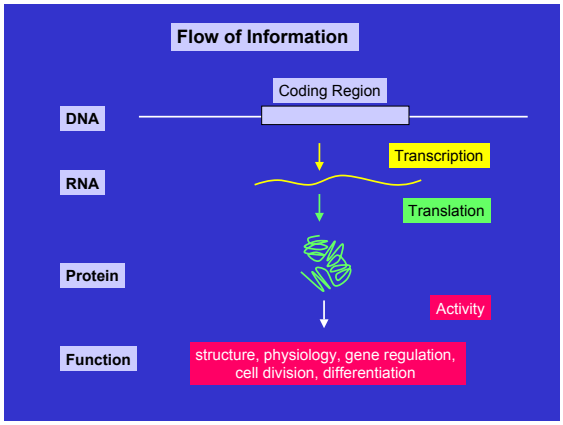
- Bio = (molecular) biology
- Informatics = computer science
- Bioinformatics = using computer science tools and techniques for solving problems in (molecular) biology
- (Loose) synonym: Computational Biology

What is Bioinformatics? (cont'd)

- Original motivation comes from molecular biology
  - Sequence analysis
  - Most accurate analysis is via experimentation ("bench work"), but expensive and time-consuming (e.g. GenBank has $> 1.1 \times 10^{11}$ base pairs from $> 1.1 \times 10^{8}$ sequences)
- Bio problems suggest computational problems, which then suggest new biological experiments

Relevant Biology Background

- Basic idea: genes (chains of nucleotides) are converted into proteins (chains of amino acids)
- Proteins are the "workhorses" of biological systems, governing metabolic processes
  - E.g. blood clotting is a process that consists of a chain reaction of numerous protein interactions



DNA and Genes

1. An organism's DNA is a (long) sequence of nucleotides (bases, residues), from {Adenine (A), Guanine (G), Cytosine (C), Thymine (T)}
2. Cellular machinery transcribes the coding regions of DNA into RNA
   - Has same alphabet, substituting U (uracil) for T
   - Non-coding regions are not transcribed

. . . ATTGATA [ATGCTGAACTACAAATTACGGCAGGCAACCGGAGCCTGGAAGTGA] TAGGA . . .

⇓

AUGCUGAACUACAAAUUACGGCAGGCAACCGGAGCCUGGAAGUGA

DNA and Genes (cont'd)

3. Then introns (non-coding subsequences) are removed, yielding mRNA
   - Adjacent triples are codons, each encoding an amino acid
4. mRNA is translated codon-by-codon into a polypeptide by ribosomes (organelles in cells' cytoplasm)
5. Proteins are comprised of one or more polypeptide chains

AUGCUG [AA] CUA [C] AAAUUACGGCAGGCAACCGGAGCCUGGAAGUGA

⇓

AUG CUG CUA AAA UUA CGG CAG GCA ACC GGA GCC UGG AAG UGA

⇓

M L L K L R Q A T G A W K [X]

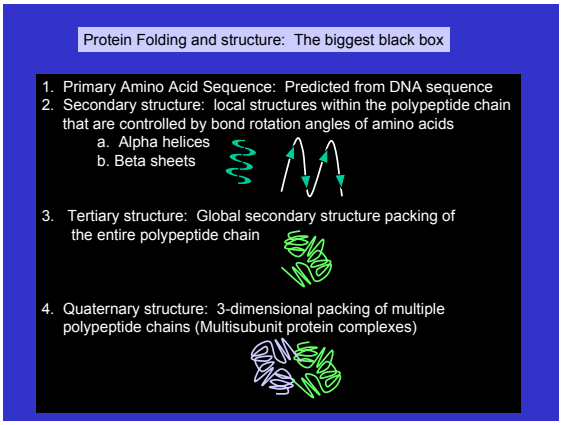
Second Position	U	C	A	G	
First position 5' end					Third position 3' end
U	Phe	Ser	Tyr	Cys	U
	Phe	Ser	Tyr	Cys	C
	Leu	Ser	STOP	STOP	A
	Leu	Ser	STOP	Trp	G
C	Leu	Pro	His	Arg	U
	Leu	Pro	His	Arg	C
	Leu	Pro	Gln	Arg	A
	Leu	Pro	Gln	Arg	G
A	Ile	Thr	Asn	Ser	U
	Ile	Thr	Asn	Ser	C
	Ile	Thr	Lys	Arg	A
	Met	Thr	Lys	Arg	G
G	Val	Ala	Asp	Gly	U
	Val	Ala	Asp	Gly	C
	Val	Ala	Glu	Gly	A
	Val	Ala	Glu	Gly	G

Genetic code is degenerate

64 codons
20 amino acids

Symbols for Amino Acids

A	Ala	Alanine	M	Met	Methionine
C	Cys	Cysteine	N	Asn	Asparagine
D	Asp	Apartic Acid	P	Pro	Proline
E	Glu	Glutamic Acid	Q	Gln	Glutamine
F	Phe	Phenylalanine	R	Arg	Arginine
G	Gly	Glycine	S	Ser	Serine
H	His	Histidine	T	Thr	Threonine
I	Ile	Isoleucine	V	Val	Valine
K	Lys	Lysine	W	Trp	Tryptophan
L	Leu	Leucine	Y	Tyr	Tyrosine



Some Fundamental Questions

- Given an organism, what is its genetic sequence?
  ⇒ Sequence assembly
- Given a sequence, what genes does it encode?
  ⇒ Gene finding
- Given a protein:
  - What is its structure?
    ⇒ Structure prediction
  - What other proteins is it related to?
    ⇒ Homology prediction/phylogeny
  - What is its function?
    ⇒ Function prediction
- All this from (mainly) only sequences of letters!

What We Will Study

- Pairwise alignment of sequences
- Multiple alignment of sequences
- Profiling (modeling) a multiple alignment
- Building phylogenetic (evolutionary) trees (time permitting)
- Predicting secondary structure and/or function of RNA and proteins (time permitting)

What We Will Not Study
(but are still interesting problems)

- Gene finding
- Inferring metabolic pathways
- Predicting tertiary structure of proteins

Topic summary due in one week!