# CSCE 471/871 Lecture 0: Administrivia

Stephen Scott

sscott@cse.unl.edu

# Welcome to 471/871!



- Check your name on the roster, or write your name if you're not listed
- Introduce yourself
  1. Who are you?
  2. What are you?
  3. Why are you here?
  4. What is one thing about you that few others know about?
- You should have the following handouts:
  1. Syllabus
  2. Copies of slides
- **Bring a laptop on Thursday!**

# CSCE 471/871 Lecture 1: Introduction

Stephen Scott

(With thanks to Andy Benson and Jitender Deogun)

sscott@cse.unl.edu

# 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 $> 1.5 \times 10^{11}$ base pairs from $> 1.6 \times 10^{8}$ sequences)
- Bio problems suggest computational problems, which then suggest new biological experiments

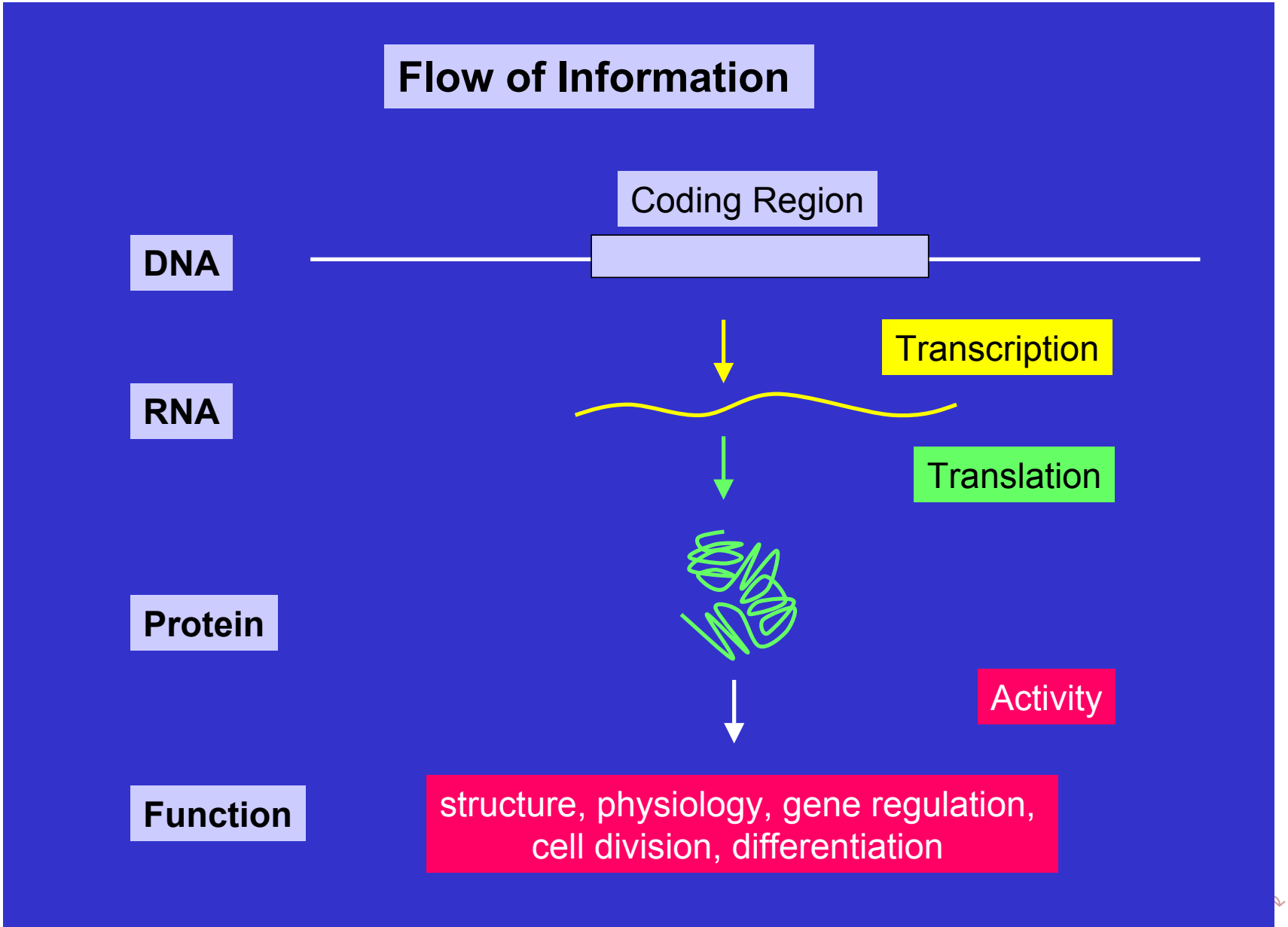
# Relevant Biology Background



- 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

# Relevant Biology Background
## Flow of Information





# Relevant Biology Background
## 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 . . .

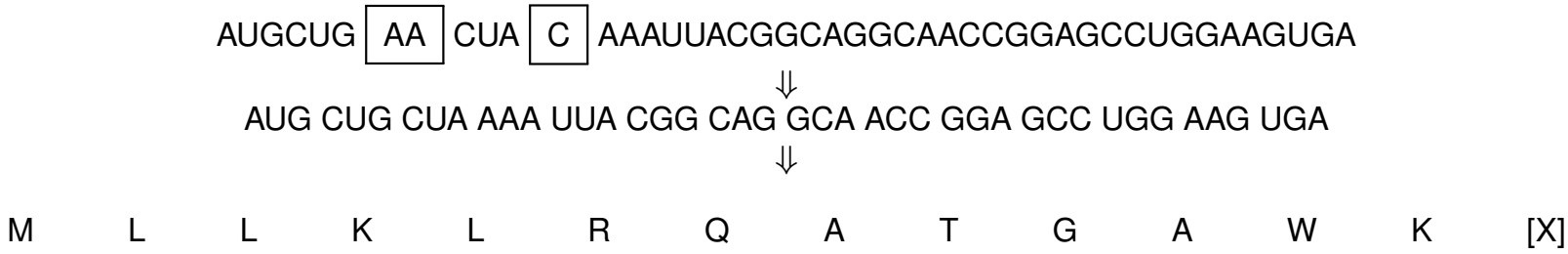
⇓

AUGCUGAACUACAAAUUACGGCAGGCAACCGGAGCCUGGAAGUGA

# Relevant Biology Background
## 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



# Relevant Biology Background
## Translation



| First position 5' end | Second Position U | Second Position C | Second Position A | Second Position G | 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

# Relevant Biology Background

## Symbols for Amino Acids



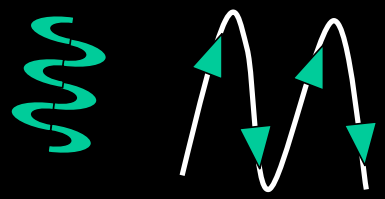
| | | | | | |
|---|---|---|---|---|---|
| A | Ala | Alanine | M | Met | Methionine |
| C | Cys | Cysteine | N | Asn | Asparagine |
| D | Asp | Apartic Acid | P | Pro | Proline |
| E | Glu | Glutamic Acid | Q | Gln | Glutamine |
| F | Phe | Phenylalanine | R | Arg | Arginine |
| G | Gly | Glycine | S | 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 |

# Relevant Biology Background
## Protein Structure



Protein Folding and structure: The biggest black box

1. Primary Amino Acid Sequence: Predicted from DNA sequence
2. Secondary structure: local structures within the polypeptide chain that are controlled by bond rotation angles of amino acids
   a. Alpha helices
   b. Beta sheets



3. Tertiary structure: Global secondary structure packing of the entire polypeptide chain

4. Quaternary structure: 3-dimensional packing of multiple polypeptide chains (Multisubunit protein complexes)

# Some Fundamental Questions



- Given an organism, what is its genetic sequence?
  $\Rightarrow$ Sequence assembly
- Given a sequence, what genes does it encode?
  $\Rightarrow$ Gene finding
- Given a protein:
  - What is its structure?
    $\Rightarrow$ Structure prediction
  - What other proteins is it related to?
    $\Rightarrow$ Homology prediction/phylogeny
  - What is its function?
    $\Rightarrow$ 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