COMP 564
Advanced Computational Biology
Methods & Research

Introduction

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Assignments & forum available on MyCourse.
Methods of Evaluation

Evaluation:

• 2 assignments (15% each)
• 1 paper presentations (10%)
• 1 project (25%)
• Final Exam (35%)
Objectives and Material

Objective: Extends the material of COMP462/561

Topics: Computational Structural & System Biology

Background: Algorithms (COMP251), Machine Learning, Probability, Programming, Basic knowledge in Molecular Biology.

Notes:

• Projects of COMP401 and COMP564 can be merged.

• We will introduce and use state-of-the-art algorithms, software and databases used in bioinformatics.
New in 2021

- Guest lecturers
- Cheminformatics & Metabolomics
- Bioinformatics of SARS-Cov-2

http://www.sbg.bio.ic.ac.uk/~mwass/casp.html

(Sun et al., BioRxiv, 2020)
Central dogma of biology

DNA → Transcription → RNA → Translation → Protein

RNA-Protein interactions → Protein-protein interactions

Function

Transfer RNA
Ribosome
Protein
DNA
RNA
Protein
The 3 components of the Bioinformatics

1. Genomic:
   Study of an organism's entire genome.
   Huge amount of data, limited to the sequence.

2. System Biology:
   Study of complex interactions in biological systems.
   High-level of representation, practical interests.

3. Computational Structural Biology:
   Study of the bio-molecule folding process.
   Lack of data in early year of bioinformatics, step toward the function, fill the gap between genomic and system biology.
(Jan. 7 – Mid Feb.) RNA bioinformatics & cheminformatics
(Mid Feb. – Mid Mar.) Protein structure and function

Dashed boxes/arrows indicate a group of arrows pointing to the same node
Mid Mar. – End Mar. : System Biology
End Mar. – Early Apr. : Paper presentations

- 10 min presentation + 5 min questions
- List of papers available at the end of September
- Participation to discussion included in grading.
(Apr. 4 – Apr. 15) Special topics
A (short) introduction to RNA structure & function
RNA world

In prebiotic world, RNA thought to have filled two distinct roles:
1. an information carrying role because of RNA's ability (in principle) to self-replicate,
2. a catalytic role, because of RNA's ability to form complicated 3D shapes.

Over time, DNA replaced RNA in its first role, while proteins replaced RNA in its second role.
**RNA classification**

**Messenger RNA:**
- Carry genetic information,
- Structure less important.

**Non-coding RNA:**
- Functional,
- Structure is important.
Cellular functions of RNA

Genetic Functions:
- Messenger RNA
- Viroids
- Transfer RNA

Enzymatic functions:
- Splicing (snRNA)
- RNA Maturation (ribonuclease P)
- Ribosomic RNA
- Guide RNA (snoRNA)
RNA structure and function

- RNAs have a 3D structure,

- This 3D structure allows complex functions,

- The variety of RNA structures allows the specific recognition of a wide range of ligands,

- Some molecules target these RNA structures (antibiotics, antiviruses):

Linezolid

Doxycyclin

Sparsomycin

Chloramphenicol
Ribonucleotides

- Nitrogenous bases
- Ribose
- Phosphate
RNA secondary structure

Central assumption: RNA secondary structure forms before the tertiary structure.

Secondary structure prediction is an important step toward 3D structure prediction.
RNA secondary structure representations

Circular

Brackets

..(((((((((..((....)))))))...(((.....))))))).))))

Dot plot

Classical
RNA secondary structure elements

- Hairpin loop
- Bulge loop
- Interior loop
- Multibranched loop
- Stem region
- Unconstrained single-stranded region