《计算生物学》开设2学分, 32学时, 7月2－27号4周，每周两次, 每次4节课, 每节课45分钟

Introduction to Computational Biology

The goal of this course is to highlight quantitatively and computational thinking in studying biological problems. The topics include analysis of biological sequences, molecular structures, and interaction networks. A diverse set of model formulations and algorithm solutions will be introduced. Students will gain exposure to basic concepts in probabilistic modeling, dynamic programming, optimization, linear algebra, computational geometry, knot theory, computational topology, stochasticity, and numerical algorithm. The course emphasizes critical thinking rather than teaching specific tools and software. In addition, several open problems will be discussed in the class. Students are expected to know some programming and are comfortable with mathematics.

1. Sequence of the working molecules of cells: proteins, RNAs, and DNAs
   1. Basics of biomolecules: Primary, secondary and tertiary structures of proteins

1.2. Detecting relationship of biomolecules by their sequences:

1.2a. Computational complexity: Can faster computer solve the problem of the world?

1.2b. Sequence alignment and dynamic programming

Global, semiglobal, and local approach

1.3b. Probabilistic model in biology and understanding results of sequence alignment.

1. Backbone of biomolecules
   1. Detecting relationship among proteins by comparing their backbone structures

2.1a. Quantifying difference in three-dimensional shapes

2.1b. Structural alignment with optimal superposition: the problem of optimization

2.2 Energy model of RNA molecules and secondary structure prediction

2.3 DNA molecules and their knottiness

2.3a. Introducton to knots and knot theory. Alexander polynomials

2.3b. Discovery of knots in biomolecules

1. The surface of biomolecule and functional sites
   1. Volumetric and surface models of proteins: approximating the physical world
   2. Geometry and topology of biomolecule when there are >10,000 atoms

Voronoi diagram, Delaunay triangulation, and alpha shapes

* 1. Algorithm for computing topological and surface properties of biomolecules.
  2. Exact computation of area and volume of biomolecules
  3. Predicting protein functions through surface computation

1. Networks of interacting biomolecules
   1. Graph structure of network of interacting molecules
   2. The principle of mass action in mesoscopic system of biochemical reactions
   3. Kinetic rates and modeling reactions using Ordinary Differential Equations
   4. Stochasticity in biochemical reactions and the framework of chemical master equation for modeling cellular fate
   5. Simulating trajectories of stochastic reactions
   6. Exact computation of probabilistic landscape of reaction network through Accurate Chemical Master Equation solutions
2. Beyond molecules and molecular networks
   1. Chromatin and chromosome folding landscape in cell nucleus
   2. Cell motility and tissue pattern formation

Textbook: Recommended but not required.

*Bhaskar* DasGupta *and Jie* Liang, Models and Algorithms for Biomolecules and Molecular Networks, January 2016 (John Wiley & Sons/IEEE), ISBN 9780470601938, Online ISBN:9781119162254 DOI:10.1002/9781119162254