CS 626 - COMPUTATIONAL MOLECULAR BIOLOGY

T/R 2: 55-4:05 Upson 205

Lecturer: Ron Elber, ron@cs.cornell.edu , 5-7416,
Walk-in-time M 10-11; W 10-11, R 9-10; F 2-3
Grade: 70% three projects; 30% take-home final (24 hours)
There is no single textbook. Detailed handouts will be provided.

(A) Sequence annotation
   a. Elements of DNA and protein sequences.
   b. Exact sequence comparison.
   c. Statistical significance of alignments.
   d. Alignments with statistical models.

(B) Modeling protein structures
   a. Elements of protein structure
   b. Comparing protein shapes
   c. Threading: matching sequences to structure
   d. Prediction of secondary structure
   e. Minestrone soups or algorithms for fold recognition

(C) "Ab-initio" modeling of protein structure
   a. Typical energy function for protein folding: reduced models, atomically detailed models, models of solvation.
   b. Global optimization techniques: Monte Carlo, Simulated annealing, smoothing algorithms
   c. Modeling side chains: Continuous space optimization, rotamer libraries, mean field approaches, dead end elimination
   d. Loop modeling using molecular dynamics and mean field approaches

(D) Modeling protein function
   a. Computing thermodynamic differences: Free energy perturbation, umbrella sampling
   b. Ligand diffusion pathways (use of a mean field approximations)
   c. Computing reaction coordinates for conformational transitions

(E) Use of existing open software
   a. Conditions for use
   b. MOIL
   c. LOOPP