MIT
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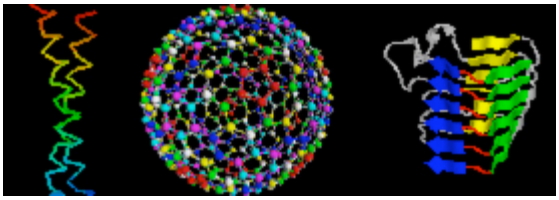

Bioinformatics Seminar

Speaker: Fabrizio Ferre, Boston College, Biology Department
Title: Disulfide connectivity prediction using secondary structure information and diresidue frequencies
Date: Monday, 18 October 2004
Time & Location:
Refreshments: 11 am in the Theory of Computation Lab at MIT's Building 32, Stata Center Room G-575
Talk: 11:30 am the Theory of Computation Lab at MIT's Building 32, Stata Center, Room G-575
URL: http://www-math.mit.edu/compbiosem/

Abstract:

Cysteine sulfhydryl groups can form strong covalent bonds (the disulfide bonds) that stabilize the tertiary and/or quaternary structures of proteins. Knowing the disulfide connectivity of a protein chain can be useful for the understanding of the protein functions and may help protein folding prediction algorithms. We describe a stand-alone software to predict disulfide bond partners in a protein given only the amino acid sequence, using a novel neural network architecture (the diresidue neural network), given input of symmetric flanking regions of N- and Cterminus half-cystines augmented with residue secondary structure (helix, coil, sheet) as well as evolutionary information. The approach is motivated by the observation of a bias in the secondary structure preferences of free cysteines and half-cystines, and by the good performance obtained using diresidue position specific scoring matrices. As calibrated by ROC curves from 4-fold cross-validation, our conditioning on secondary structure leads to a performance comparable or improved over the current state-of-the-art method. A slight drop in performance is seen when secondary structure is predicted rather than derived from three dimensional protein structures. A web engine (http://clavius.bc.edu/~clotelab/DiANNAforDBC/) allows the on-line use of this tool.

The seminar is co-hosted by Professor Peter Clote of Boston College's Biology and Computer Science Departments and MIT Professor of Applied Math Bonnie Berger. Professor Berger is also affiliated with CSAIL & HST.

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