MIT
Department of Mathematics
& The Theory of
Computation Group
At CSAIL

Bioinformatics Seminar

Speakers: Jinbo Xu, TTI
Title: A Parameterized Algorithm for Protein Structure Alignment
Date: Monday, 15 May 2006
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:

This talk presents a parameterized algorithm for aligning two protein structures, in the case where one protein structure is represented by a contact map graph and the other by a contact map graph or a distance matrix. If the sequential order of alignment is not required, the time complexity is polynomial in the protein size and exponential with respect to two parameters $\frac{D_u}{D_l}$ and $\frac{D_c}{D_l}$, which usually can be treated as constants. In particular, D_u is the distance threshold determining if two residues are in contact or not, D_c is the maximally allowed distance between two matched residues after two proteins are superimposed, and D_l is the minimum inter-residue distance in a typical protein. This result indicates that if both $\frac{D_u}{D_l}$ and $\frac{D_c}{D_l}$ are small enough, then there is a polynomial-time approximation scheme for the non-sequential protein structure alignment problem. Empirically, both $\frac{D_u}{D_l}$ and $\frac{D_c}{D_l}$ are very small and can be treated as constants. This result clearly demonstrates that the hardness of the contact-map based protein structure alignment problem is related not to protein size but to several parameters, which depend on how the protein structure alignment problem is modeled. The result is achieved by decomposing the protein structure using tree decomposition and discretizing the rigid-body transformation space.

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