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Abstracts of Plenary and Invited Lectures

Section:

16. Applications

Section 16 b: (Non-Continuum) Applied Area

1991 MS Classification: Mathematical Biology
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Sequence-based Methods for Protein Folding

One of the most important and challenging problems in computational biology is that of predicting the three-dimensional structure or shape of a protein from its amino acid sequence. As a first step to tackling this problem, many researchers have focused on the structural motif recognition problem: given a known local three-dimensional structure, or motif, determine whether this motif occurs in a given amino acid sequence.
In this talk, I will present algorithms that use probabilistic techniques to improve existing methods for recognizing protein structural motifs. These algorithms are particularly effective at eliminating false positives found by previous methods without introducing false negatives.
We have implemented these algorithms and have tested them on 2-stranded and 3-stranded coiled coils. The coiled coil motif has many important biological roles; for example, it is found in some DNA binding proteins and is thought to play a role in the membrane fusion of retroviruses. Our algorithms have been codified in three programs: PairCoil, which is significantly better than existing methods at identifying 2-stranded coiled coils; MultiCoil, which identifies and distinguishes between 3-stranded and 2-stranded coiled coils; LearnCoil, which is particularly effective in scenarios where sufficiently diverse examples of a motif are not known.
Finally, I will talk about some of the biological implications of our work. In particular, we have identified interesting domains in the envelope proteins of retroviruses such as the influenza virus, Moloney murine leukemia virus, and HIV, as well as in a large class of proteins involved in sensory signaling.
(Portions of this work are joint with Peter S. Kim, Ethan Wolf, Mona Singh, David Wilson, and Andrea Cochran.)