

Public Abstract

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Department:Computer Science

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Title:A Novel Framework for Protein Tertiary Structure Prediction

Proteins are one of the most important molecules in the life processes. The structure of a protein is essential in understanding the function of a protein at the molecular level. Due to rapid progress in sequencing technologies, the gap between the proteins whose structure is known and the proteins whose structure needs to be characterized is rapidly increasing. To address this problem, we are developing a novel framework to computationally predict many aspects of proteins like secondary structure, solvent accessibility, contact map and finally, the tertiary structure itself. We have applied various computational techniques including the fuzzy k-nearest neighbor algorithm, the multi-dimensional scaling method, and the least-squares minimization, in the structure predictions. Our framework uses the evolutionary information more effectively than traditional template based methods, while it has a better potential to utilize the information in PDB than the other evolutionary information based methods. Our methods show better performance in prediction accuracy and computational time than many other tools.