Towards Automated NMR Protein Structure Determination

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Abstract

Protein three-dimensional structure determination is the key towards the understanding of the function of the human body. Nuclear Magnetic Resonance (NMR) is one of the two main methods for protein structure determination. Currently it takes weeks to months of human labor to determine a protein structure after NMR experiments. If we could fully automate this process, this would significantly speedup the structural biology research. In this talk, we will identify the key obstacles in NMR data processing and propose solutions by computational methods. We will discuss our efforts on developing signal processing techniques for the peak picking problem, optimization techniques for the resonance assignment problem, and machine learning techniques for the structure calculation problem. Each of these methods subtly handles the noise and imperfection of the others and significantly outperforms the state-of-the-art approaches. As a proof of concept, we combine the proposed methods into a system, AMR, which has succeeded in determining high resolution protein structures from a small set of NMR spectra, in a day.

The Biography

Xin Gao is an assistant professor in Computer, Electrical and Mathematical Sciences and Engineering Division at KAUST, and an adjunct faculty member at University of Waterloo. He leads the Structural and Functional Bioinformatics group at KAUST. Before he moved to KAUST, he was a Lane Fellow in Lane Center for Computational Biology in School of Computer Science at Carnegie Mellon University, US. He received the Ph.D. degree in Computer Science from the University of Waterloo in 2009, and the B.Sc. degree in Computer Science from Tsinghua University, China in 2004.