

## Probabilistic Graphical Model for Protein Structure Prediction

### Abstract:

If we know the primary sequence of a protein, can we predict its three-dimensional structure by computational methods? This is one of the most important and difficult problems in computational molecular biology and has tremendous implications for protein functional study and drug discovery.

Existing computational methods for protein structure prediction can be broadly classified into two categories: template-based modeling (i.e., protein threading/homology modeling) and template-free modeling (i.e., ab initio folding). Template-based modeling predicts structure of a protein using experimental structures in the Protein Data Bank (PDB) as templates while template-free modeling predicts protein structure without depending on a template.

This talk will present new probabilistic graphical models for knowledge-based protein structure prediction. In particular, this talk will present a regression-tree-based Conditional Random Fields (CRF) method for template-based modeling and a Conditional Random Fields/Conditional Neural Fields (CRF/CNF) method for template-free modeling. Experimental results indicate that our template-based method performs extremely well, especially on hard template-based modeling targets and our template-free method is also very promising for mainly-alpha proteins.

### Short Bio:

Dr. Jinbo Xu currently is an assistant professor at the Toyota Technological Institute at Chicago (a computer science institute on the campus of the University of Chicago). He is also a visiting scientist at the CSAIL of the Massachusetts Institute of Technology. Dr. Xu received his PhD in Computer Science from the University of Waterloo and then spent one year as a Postdoctoral Fellow in the Department of Mathematics, MIT. Dr. Xu's primary research interest is computational biology and bioinformatics including analysis and modeling of biological sequences, structures and networks. His RaptorX/RAPTOR programs have been ranked very top in several CASP (Critical Assessment of Structure Prediction) events, the most well-known competitions in the field of protein

structure prediction. Dr. Xu was also invited to speak at the CASP meetings and publish papers in the CASP special issues.