

Jinbo Xu

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Education and Training

Department of Mathematics, Massachusetts Institute of Technology
Postdoctoral Fellow, 2004--2005 (Supervisor: Prof. Bonnie Berger)

School of Computer Science, University of Waterloo, Canada
Ph.D. in Computer Science, 1999--2003 (Supervisor: Profs. Ming Li and Prabhakar Ragde)

Institute of Computing Technology, Chinese Academy of Sciences, China
Master of Science in Computer Science, 1996--1999

Department of Computer Science, University of Science and Technology of China
Bachelor of Science in Computer Science, 1991--1996

Employment and Affiliations

2005-present Assistant Professor, Toyota Technological Institute at Chicago
2005-present Assistant Professor (part-time), University of Chicago
2006-present Research Affiliate, Massachusetts Institute of Technology
2004-present Adjunct Assistant Professor, University of Waterloo
2003-2004 Research Assistant Professor, University of Waterloo

Research Interest

Bioinformatics and computational biology including analysis and modeling of biological sequences, structures and networks; machine learning and pattern recognition; optimization algorithm

Honors and Fellowships

2010 RaptorX ranked No.2 in CASP9 among ~80 servers (in terms of GDT-TS);
The best for the 50 hardest TBM (template-based modeling) targets;
RaptorX voted by the CASP9 community as one of the most interesting
and innovative methods

2010 Invited talks (one regular and two short) at the CASP9 meeting

2009 Best poster award at RECOMB 2009

2009 Invited paper to the CASP8 (The 8th Critical Assessment of Structure

	Prediction) special issue
2008	RAPTOR officially ranked No.2 in CASP8 among ~75 servers
2008	CASP8 travel fellowship
2008	Best poster award at the CASP8 conference with Tobin Sosnick group
2004-2005	PMMB (Program in Mathematics Molecular Biology) fellowship
2004	Invited talk at CASP6 due to RAPTOR's superior performance
2003	PhD thesis nominated for ACM Doctoral Dissertation Award and NSERC Doctoral Prize
2002	Invited paper to the CASP5 special issue; RAPTOR ranked first in the fold recognition category among all servers and voted as the most novel method
1999-2003	International Student Scholarship, the University of Waterloo
1995	Second prize in National Collegiate Contest on Mathematical Modeling
1990	First prize in China High School Mathematical Contest; No.1 in Jiangxi province

student honors

2010 My PhD student Mr. Jian Peng won the prestigious Microsoft Research PhD Fellowship in 2010 (only 10 out of 176 applicants were awarded.)

Grants

1. Jinbo Xu. NSF/ABI "Algorithm and web server for low-homology protein threading". (total cost ~\$408k, July 2010-June 2013)
2. Jinbo Xu. NIH/NIGMS (R01GM089753-01) "New computational methods for data-driven protein structure prediction". (total cost ~\$1.35M, May 2010-April 2015)
3. Tobin Sosnick (PI), Karl Freed, and Jinbo Xu. NIH/NIGMS (1R01GM081642-01) "Protein structure refinement using novel move set", 08/2007-08/2010.
4. Bonnie Berger (PI), Jinbo Xu and Jadwiga Bienkowska. NIH/NIGMS (1R01GM081871-01A1) "Prediction of protein interactome", 12/2007-12/2012.

The following two grants provide computational resources support:

5. Jinbo Xu. (NSF-sponsored) TeraGrid TG-MCB100062 (2M CPU hours, 2010)
6. Jinbo Xu. (NSF-sponsored) TeraGrid TG-CCR100005 (200k CPU hours, 2009)

Pending Grants

1. Tobin Sosnick, Karl Freed, and Jinbo Xu (Multiple PI Leadership). NIH/NIGMS, "Integrated template and free modeling of clinically important S. aureus proteins".
2. Jinbo Xu. DOE, "A highly-scalable tool for multiple protein sequence and structure alignment".

Professional Activities

1. Ad hoc member for NIH ZRG1 Biological Chemistry and Macromolecular Biophysics (BCMB)-A (96) Special Emphasis Panel (2009/07) and NIH MSFD study section (2009/10, 2010/10)
2. Panelist for NSF Bio division (2010/05) and ad hoc reviewer for NSF Pan-American Advanced Studies Institutes Program (2009/02)
3. Ad hoc reviewer for Israel Science Foundation 2010
4. Program committee member for RECOMB2011, ISMB2010, RECOMB2010, IEEE BIBM10, IEEE BIBM09, ICMLA09, DTMBIO09, IEEE BIBM08, BIDM07, IEEE BIBE07, and ICMLA07
5. Program co-chair of the Bioinformatics and Computational Biology workshop, the Eighth International Conference on High-Performance Computing in Asia-Pacific Region (HPC-Asia 2005)
6. Reviewer for PNAS, Bioinformatics, IEEE/ACM TCBB, JCB, BMC Bioinformatics, JCB, Journal of Combinatorial Optimization, Journal of Proteome, Protein Engineering, Algorithmica, Pattern Recognition Letter, Mathematical Biosciences, Journal of Mathematical Biology, SIAM Journal of Computing, ACM-SIAM Symposium on Discrete Algorithms (SODA 2007), Journal of Molecular Biology

Mentorship

1. Jian Peng, Feng Zhao, Zhiyong Wang, Xing Xu and Jianzhu Ma (PhD students)
2. Haipeng Wang and Sheng Wang (postdocs)
3. Xin Gao (co-supervised with Prof. Ming Li, now faculty at KAUST)
4. Shuaicheng Li (co-supervised with Prof. Ming Li, now a postdoc at UC Berkeley)
5. Morten Kallberg (summer intern in 2010, now a PhD student at the University of Illinois)
6. Beckett W. Sterner (summer intern in 2007, now a PhD student at U Chicago)
7. Xu Zhang (summer intern in 2006, now working at Amazon)
8. Xishu Wang (summer intern in 2008)

Peer-reviewed Publications (in reverse chronological order)

(The * symbol indicates corresponding/co-corresponding author. I merge conference and journal publications in a single list since the listed conference publications are also peer-reviewed and the conferences in which these publications appear have low acceptance rate.)

Under Review

1. Jian Peng and **Jinbo Xu***. A multiple-template approach to protein threading. PROTENS, 2010 (revision submitted after first review)

Published or In Press

2. Zhiyong Wang, Jian Peng, Feng Zhao and **Jinbo Xu***. Protein 8-class secondary structure prediction using conditional neural fields. IEEE BIBM 2010. In Press.
3. Raghavendra Hosur, **Jinbo Xu**, Jadwiga Bienkowska, and Bonnie Berger. iWRAP: An interface threading approach with application to prediction of cancer related protein-protein interactions. Journal of Molecular Biology, December 2010.
4. Rohit Singh, Daniel Park, **Jinbo Xu**, Raghavendra Hosur and Bonnie Berger. Struct2Net: a Web-Service to Predict Protein-Protein Interactions Using a Structure-based Approach. NAR web server issue, 2010. (**The first three authors equally contribute to this paper.**)
5. Feng Zhao, Jian Peng and **Jinbo Xu***. Fragment-free Approach to Protein Folding Using Conditional Neural Fields. Bioinformatics (Proceedings of ISMB 2010), Vol. 26, pp. i294-i300, 2010.
6. Jian Peng and **Jinbo Xu***. Low-homology protein threading. Bioinformatics (Proceedings of ISMB 2010), Vol. 26, pp. i310-i317, 2010.
7. Feng Zhao, Jian Peng, Joe DeBartolo, Karl F. Freed, Tobin R. Sosnick and **Jinbo Xu***. A probabilistic and continuous model of protein conformational space for template-free modeling. Journal of Computational Biology, 2010 Jun;17(6):783-98..
8. Jian Peng, Liefeng Bo and **Jinbo Xu**. Conditional Neural Fields. NIPS 2009.
9. Xin Gao, Dongbo Bu, **Jinbo Xu** and Ming Li. Improving consensus contact prediction via server correlation reduction. BMC Structural Biology 2009, 9:28
10. **Jinbo Xu***, Jian Peng and Feng Zhao. Template-based and free modeling by RAPTOR++ in CASP8. The CASP8 special issue of PROTEINS, 2009. (**invited paper**)
11. Jian Peng and **Jinbo Xu***. Boosting protein threading accuracy. In the Proceedings of the 13th International Conference on Research in Computational Molecular Biology (RECOMB), Lecture Notes in Computer Science, Vol. 5541, pp. 31-45, 2009. Springer.
12. Feng Zhao, Jian Peng, Joe DeBartolo, Karl F. Freed, Tobin R. Sosnick and **Jinbo Xu***. A probabilistic graphical model for ab initio folding. In the Proceedings of the 13th International Conference on Research in Computational Molecular Biology (RECOMB), Lecture Notes in Computer Science, Vol. 5541, pp. 59-73, 2009. Springer.
13. Shuaicheng Li, Dongbo Bu, **Jinbo Xu*** and Ming Li. Fragment-HMM: A new approach to protein structure prediction. Protein Science, 2008 Nov;17(11):1925-34.
14. Feng Zhao, ShuaiCheng Li, Beckett W. Sterner and **Jinbo Xu***. Discriminative learning for protein conformation sampling. PROTEINS: Structure, Function and Bioinformatics, 2008 Oct; 73(1):228-40.
15. Shuaicheng Li, Dongbo Bu, Xin Gao, **Jinbo Xu*** and Ming Li. Designing protein structural alphabets, 16th Annual International Conference Intelligent Systems for Molecular Biology (ISMB). Also appears at Bioinformatics, 2008 24(13):i182-i189
16. Rohit Singh, **Jinbo Xu** and Bonnie Berger. Global Alignment of Multiple Protein-Protein Interaction Networks. PNAS, 2008 Sep 2;105(35):12763-8.
17. Jing Zhang, Xin Gao, **Jinbo Xu*** and Ming Li. Rapid Protein Side-Chain Packing Using Local Backbone Information. In the Proceedings of the 11th International Conference on Research in Computational Molecular Biology (RECOMB), 285-299. Lecture Notes in Computer Science 4955 Springer 2008.

18. Ben Boyerinas, Sun-Mi Park, Noam Shomron, Cydney B. Nielsen, Christine Feig, **Jinbo Xu**, Christopher B. Burge and Marcus E. Peter. Identification of let-7-regulated Oncofetal Genes for Human Cancer. *Cancer Research*, 2008 Apr 15; 68(8):2587-91.
19. Bonnie Berger, Rohit Singh and **Jinbo Xu**. Graph Algorithms for Biological Systems Analysis. In the Proceedings of the nineteenth annual ACM-SIAM Symposium on Discrete Algorithms (SODA), 2008. (**invited paper and authors ranked alphabetically**)
20. Rohit Singh, **Jinbo Xu** and Bonnie Berger. Global Alignment of Multiple Protein Interaction Networks. In the Proceedings of Pacific Symposium in Biocomputing 13:303-314, 2008. Hawaii, USA.
21. **Jinbo Xu**. Solving the Contact Map Overlap Problem via Tree Decomposition and a DEE-Like Pruning Strategy, in the Proceedings of the 46th IEEE Conference on Decision and Control, December 2007. Orlando, USA. (**invited paper**)
22. Xin Gao, Dongbo Bu, Shuai Cheng Li, **Jinbo Xu*** and Ming Li. FragQA: predicting local fragment quality of a sequence-structure alignment. In the Proceedings of the 17th International Conference on Genome Informatics (GIW), December 2007. (**best paper award**)
23. Xin Gao, Dongbo Bu, ShuaiCheng Li, Ming Li, and **Jinbo Xu***. Consensus Contact Prediction by Linear Programming, Life Science Society Computational Systems Conference, August 2007. Stanford, USA.
24. Jianbo Qian, Shuai Cheng Li, Dongbo Bu, Ming Li and **Jinbo Xu**. Finding Compact Structural Motifs in Many Proteins, Combinatorial Pattern Matching (CPM), July 2007. London, Canada.
25. Dongbo Bu, Shuaicheng Li, Xin Gao, Libo Yu, **Jinbo Xu** and Ming Li. Consensus Approaches to Protein Structure Prediction. Book Chapter in Machine Learning in Bioinformatics, Eds: Yan-Qing Zhang and Jagath C. Rajapakse, John Wiley & Sons, 2007.
26. Rohit Singh, **Jinbo Xu** and Bonnie Berger. Pairwise Global Alignment of Protein Interaction Networks By Matching Neighborhood Topology. In the Proceedings of the 11th International Conference on Research in Computational Molecular Biology (RECOMB), 16-31. Lecture Notes in Computer Science 4453 Springer 2007.
27. **Jinbo Xu***, Libo Yu and Feng Jiao. Protein Structure Prediction Using Threading. Book Chapter in Protein Structure Prediction: Methods and Protocols, Humana Press, 2007.
28. **Jinbo Xu***, Bonnie Berger. Fast and Accurate Algorithms for Protein Side-Chain Packing. *The Journal of the ACM*, 53(4):1-25, 2006. (**invited paper. JACM provides coverage of the most significant work in computer science.**)
29. **Jinbo Xu**, Daniel Brown, Ming Li and Bin Ma. Optimizing multiple spaced seeds for homology search. *Journal of Computational Biology*, 13(7):1355-1368, 2006.
30. Feng Jiao, **Jinbo Xu***, Libo Yu and Dale Schuurmans. Protein Fold Recognition Using the Gradient Boost Algorithm. Life Science Society Computational Systems Bioinformatics (CSB), 2006. Stanford, USA.

31. **Jinbo Xu***, Feng Jiao and Bonnie Berger. A Parameterized Algorithm for Protein Structure Alignment. In the Proceedings of the 10th International Conference on Research in Computational Molecular Biology (RECOMB), Lecture Notes in Bioinformatics 3909, 488-499. Springer 2006.
32. Rohit Singh, **Jinbo Xu** and Bonnie Berger. Struct2Net: Integrating Structure into Protein-Protein Interaction Prediction. Pacific Symposium on Biocomputing 2006:403-414, Hawaii, USA.
33. **Jinbo Xu**. Protein Fold Recognition by Predicted Alignment Accuracy. IEEE/ACM Trans. on Computational Biology and Bioinformatics. 2(2):157-165, 2005.
34. **Jinbo Xu**, Feng Jiao and Bonnie Berger. A Tree-Decomposition Approach to Protein Structure Prediction. Computational Systems Bioinformatics (CSB), 2005. Stanford, USA.
35. **Jinbo Xu**. Rapid Protein Side-Chain Packing via Tree Decomposition. In the Proceedings of the 9th International Conference on Research in Computational Molecular Biology (RECOMB), Lecture Notes in Computer Science, Vol. 3500, pp. 423-439, 2005. Springer. (**The extended version of this paper was invited to the Journal of the ACM.**)
36. **Jinbo Xu**, Libo Yu and Ming Li. Consensus Fold Recognition by Predicted Model Quality. Asia-Pacific Bioinformatics Conference 2005:73-83, Singapore.
37. Thomas Tang, **Jinbo Xu** and Ming Li. Discovery of Sequence-Structure Motifs from Protein Segments and Two Applications. Pacific Symposium on Biocomputing 2005. Hawaii, USA.
38. **Jinbo Xu**, Ying Xu and Ming Li. Protein Threading by Linear Programming: Theoretical Analysis and Computational Results, Journal of Combinatorial Optimization, 8(4):403-418, 2004.
39. **Jinbo Xu**, Daniel Brown, Ming Li and Bin Ma. Optimizing multiple spaced seeds for homology search. Combinatorial Pattern Matching 2004, Istanbul, Turkey.
40. **Jinbo Xu**, Ying Xu, Dongsup Kim and Ming Li. RAPTOR: Optimal Protein Threading by Linear Programming, Journal of Bioinformatics and Computational Biology, 1(1):95-118, 2003. (**invited paper**)
41. **Jinbo Xu*** and Ming Li. Assessment of RAPTOR's linear programming approach in CAFASP3, the CASP5 special issue, PROTEINS: Structure, Function and Genetics. 2003; 53 Suppl 6:579-84. (**invited paper**)
42. **Jinbo Xu**, Ying Xu, Guohui Lin, Dongsup Kim and Ming Li. Protein Structure Prediction By Linear Programming, Pacific Symposium on Biocomputing 2003: 264-275, Hawaii, USA.
43. **Jinbo Xu**. Speed up LP Approach to Protein Threading via Graph Reduction, in the Proceedings of the 3rd International Workshop on Algorithms in Bioinformatics (WABI), Lecture Notes in Computer Science Vol. 2812, pp. 374-388, 2003. Springer.
44. Zhi-Zhong Chen, Tao Jiang, Guo-Hui Lin, Jianjun Wen, Dong Xu, **Jinbo Xu** and Ying Xu. Approximation Algorithms for NMR Spectral Peak Assignment, Theoretical Computer Science, 299:211-229, 2003. (**authors ranked alphabetically**)

Invited Talks

(This list does not include my conference talks for an accepted paper.)

1. RaptorX: low-homology protein threading and multiple-template threading. CASP9, Dec 2010.
2. Probabilistic models for protein sequence/structure alignment with application to protein modeling. MIT, Feb 2011.
3. Probabilistic models for protein sequence/structure alignment with application to protein modeling. CMU, Feb 2011.
4. Probabilistic models for protein sequence/structure alignment with application to protein modeling. McGill University, Feb 2011.
5. Probabilistic graphical models for protein structure prediction. Dartmouth College, April 2010.
6. Optimization techniques for protein structure prediction. The Institute of Illinois Technology, March 2010.
7. Protein threading by nonlinearly combining evolutionary and non-evolutionary information. The University of Minnesota, 2009.
8. Protein threading by nonlinearly combining evolutionary and non-evolutionary information. MIT, 2009.
9. Linear programming approach to protein structure prediction. INFORMS Annual Meeting, October 2008.
10. Graph Algorithms for Biological Systems Analysis. SIAM on Discrete Mathematics, June 2008.
11. Global Alignment of Multiple Protein Interaction Networks. The University of Illinois at Chicago, 2008.
12. Protein Conformation Sampling Using Conditional Random Fields, MIT, 2008.
13. Graph Algorithms for Protein Structure Alignment. The 46th IEEE Conference on Decision and Control, December 2007.
14. Knowledge-based Protein Structure Prediction. Institute of Computing Technology, Chinese Academy of Sciences, March 2007. (Distinguished Lecture)
15. Knowledge-based Protein Structure Prediction. Tsinghua University, March 2007.
16. Knowledge-based Protein Structure Prediction. Microsoft Research in Asia, March 2007.
17. Knowledge-based Protein Structure Prediction. Toyota Technological Institute at Japan, April 2007.
18. Protein Side Chain Packing via Tree Decomposition. University of Waterloo, August 2006.
19. A Parameterized Algorithm for Protein Structure Alignment. University of Waterloo, July 2006.
20. A Parameterized Algorithm for Protein Structure Alignment. MIT, May 2006.
21. Knowledge-based Protein Structure Prediction. Northwestern University, May 2006.
22. A Parameterized Algorithm for Protein Structure Alignment. University of Illinois at Chicago, November 2005.

23. Fast and Accurate Algorithms for Protein Side-Chain Packing. Boston University, October 2005.
24. Rapid Protein Side-Chain Packing via Tree Decomposition. DIMACS Workshop on Information Processing by Protein Structures in Molecular Recognition. June 13-14, 2005.
25. RAPTOR: protein threading by linear programming. SIAM mini-symposium, SIAM Conference on Control and Its Applications. New Orleans, LA, July 11-14, 2005.
26. ACE: consensus method to fold recognition. CASP6, Italy. December 2004. (an invitation to our ACE group)
27. Protein Structure Prediction by Linear Programming. School of Medicine, University of Western Ontario, 2004.
28. Protein Structure Prediction. The Interdisciplinary Coffee Talk Society, University of Waterloo, 2003.