

# Jinbo Xu

Toyota Technological Institute at Chicago  
6045 S. Kenwood Ave.  
Chicago, IL 60637

Email: [jinboxu@gmail.com](mailto:jinboxu@gmail.com)  
Fax: 773 834 9881  
Phone: 773 359 3721  
URL: <http://ttic.uchicago.edu/~jinbo>

## Education and Training

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

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

2014-	Senior Fellow, Computational Institute (at the University of Chicago)
2012-present	Associate Professor, Toyota Technological Institute at Chicago (at the University of Chicago)
2005-2012	Assistant Professor, Toyota Technological Institute at Chicago
2006-2012	Assistant Professor (part-time), Department of Computer Science, University of Chicago
2006-present	Research Affiliate, Massachusetts Institute of Technology
2004-2010	Adjunct Assistant Professor, University of Waterloo
2003-2004	Research Assistant Professor, University of Waterloo

## Primary research and teaching interests

Machine Learning, Optimization, Big Data, Bioinformatics and Computational Biology

## Personal Statement

My research lies in the interface of combinatorial and numerical optimization, statistical machine learning, and some emerging data-rich areas such as computational biology. I am interested in studying theoretically sound and empirically efficient optimization and machine learning algorithms to analyze, interpret, and integrate high volumes of multi-dimensional and heterogeneous data and based upon which building effective mathematical models. On one hand, I would like to develop computational methods for addressing a specific challenging problem by taking full advantage of domain-specific knowledge and data. On the other hand, I would like to study novel and scalable optimization/machine learning algorithms that are widely applicable. I have been

focusing on analyzing the massive sets of biological sequence, structure and network data and developed several popular bioinformatics tools. In particular, I am known for having designed a protein structure prediction program RAPTOR/RaptorX, which has been ranked very top from CASP5 to CASP10 (Critical Assessment of Structure Prediction), the most well-known competitions in the field of computational biology. I am also known for the IsoRank algorithm for comparative analysis of protein-protein interaction networks. Finally, I am open to collaboration with people in optimization/machine learning, high-performance computing, social science, medicine, and financial engineering.

## Major Honors

2012 Alfred P. Sloan Research Fellowship

2012 NSF CAREER Award

My protein structure prediction program RAPTOR/RaptorX constantly ranked very top from CASP5 to CASP10 (Critical Assessment of Structure Prediction). In particular, it was ranked No. 1 for the hardest template-based modeling targets and voted among the most innovative and interesting methods in CASP5, CASP9 and CASP10. I have been invited to give quite a few talks in the CASP meetings and publish several papers on the CASP special issues.

## Other Honors

2014 ACM SIGBio best student paper award with student Zhiyong Wang and Prof. Xinghua Shi

2014 Best paper award at RECOMB2014

2014 Warren DeLano Award for Structural Bioinformatics and Computational Biophysics at ISMB 3DSIG 2014 (with PhD student Mr. Jianzhu Ma)

2013 Best poster award in the 2013 Zing conference for protein and RNA structure

2012 Warren DeLano Award for Structural Bioinformatics and Computational Biophysics in ISMB 3DSIG 2012 (with postdoc Dr. Sheng Wang)

2010 Former PhD student Jian Peng won the prestigious Microsoft Research PhD Fellowship in 2010 (only 10 out of 176 applicants were awarded) and 2011 CROI Young Investigator Award

2009 Best poster award at RECOMB 2009

2008 Best poster award at the CASP8 conference (with Tobin Sosnick)

2004-2005 PMMB (Program in Mathematics Molecular Biology) fellowship

1995 Second prize in National Collegiate Contest in Mathematical Modeling

1990 First prize in China High School Mathematics Contest; No.1 in Jiangxi province

## Grants (My own research expenditure > \$3 millions)

1. Jinbo Xu. NSF/BIO DBI-1262603. *Continued development of RaptorX for protein structure and function prediction*. Total cost ~\$540k, 7/1/2013-6/30/2016

2. Jinbo Xu. NSF/CCF AF-1149811 (CAREER award). *Exact and approximate algorithms for 3D structure modeling of protein-protein interactions*. Total cost ~\$500k, July 2012-June 2017
3. Jinbo Xu. NIH R01GM089753. *New computational methods for data-driven protein structure prediction*. Total cost ~\$1.35m, May 2010-April 2015
4. Jinbo Xu. NSF/BIO DBI-0960390: *Algorithm and web server for low-homology protein threading*. Total cost ~\$408k, July 2010-June 2013
5. Tobin Sosnick (PI), Karl Freed, and Jinbo Xu. NIH R01GM081642. *Protein structure refinement using novel move set*. My share ~\$200k, 08/2007-08/2010
6. Bonnie Berger (PI), Jinbo Xu and Jadwiga Bienkowska. NIH R01GM081871A1. *Prediction of protein interactome*. My share ~\$100k, 12/2007-12/2012

The following grants provide computational resources support:

7. Jinbo Xu. TeraGrid TG-MCB100062 (1 million CPU hours, 2012)
8. Jinbo Xu. TeraGrid TG-MCB100062 (3.7 million CPU hours, 2010- 2011)
9. Jinbo Xu. TeraGrid TG-CCR100005 (200k CPU hours, 2009)

## Professional Activities

1. Associate editor for IEEE/ACM TCBB. Area chair for ISMB2014 and ACM-BCB 2012. Program co-chair of the Bioinformatics and Computational Biology workshop, the 8th International Conference on High-Performance Computing in Asia-Pacific Region (HPC-Asia 2005)
2. Reviewer for NIH ZRG1 Biological Chemistry and Macromolecular Biophysics (BCMB)-A (96) Special Emphasis Panel (2009/07), NIH MSFD study section (2009/10, 2010/10, 2015/6), NIH BDMA study section (2011/10), NIH K99 (2012-2013)
3. Panelist for NSF CISE (2012/04) and Bio division (2010/05), ad hoc reviewer for NSF ABI (2011) and ad hoc reviewer for NSF Pan-American Advanced Studies Institutes Program (2009/02); Ad hoc reviewer for ISF (Israel Science Foundation) (2010, 2011)
4. Program committee member for ICML (2012-2014), RECOMB (2010-2012,2014), ISMB (2010-2014), IEEE BIBM (2008-2014), ACM BCB (2010-2012), ICMLA(2007-2012), BIDM07 and IEEE BIBE07
5. Reviewer for PNAS, Bioinformatics, IEEE/ACM TCBB, JBCB, BMC Bioinformatics, JCB, Journal of Combinatorial Optimization, Journal of Proteome, PROTEINS, 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, Biophysics Journal

## Mentorship

1. Current PhD students: Lifu Tu, Qingming Tang, Somaye Hashemifar, Siqi Sun, and Jianzhu Ma
2. Former PhD students and postdocs
  - 1) Jian Peng (PhD student, now a tenure-track faculty member at UIUC CS)
  - 2) Feng Zhao (PhD student, now in Wall Street)

- 3) Zhiyong Wang (PhD student, now in Google)
- 4) Sheng Wang (postdoc, now a research scientist at UChicago BSD)
- 5) Xiaohui Chen (summer intern and postdoc, now a tenure-track faculty member at UIUC Statistics)
- 6) Haipeng Wang (postdoc)
- 7) Xin Gao (co-supervised with Prof. Ming Li, now a tenure-track faculty member at KAUST)
- 8) Shuaicheng Li (co-supervised with Prof. Ming Li, now a tenure-track faculty member at Hong Kong City Univ.)

### 3. Summer interns

Gohar Margaryan (2011-2013), Mengfei Cao (2013), Morten Kallberg (2010, first job at Illumina), Xishu Wang (2008, first job in finance industry), Beckett W. Sterner (2007, now postdoc at Field Museum), Xu Zhang (2006, first job at Amazon)

## Publications

In Computer Science, top conference papers have lower acceptance rate than many top journals and are highly regarded. NIPS and AISTATS are top machine learning conferences. RECOMB and ISMB are two top computational biology conferences and in total accept ~80 regular papers each year. JACM is the most prestigious (theory-oriented) computer science journal, which publishes ~30 papers a year. Since 2005, my group in total has published 15 papers at the RECOMB and ISMB main conferences, 1 NIPS and 6 AISTATS (AI and Statistics) papers and 1 JACM paper. Most of my RECOMB and ISMB papers are the application of machine learning and optimization algorithms to biology problems.

### **Peer-reviewed conference papers** (\* indicates corresponding author)

1. Qingming Tang, Siqi Sun and Jinbo Xu\*. *Learning Scale-Free Networks by Dynamic Node Specific Degree Prior*. International Conference on Machine Learning (ICML), 2015
2. Jianzhu Ma, Qingming Tang and Jinbo Xu\*. *Structure Learning Constrained by Node-Specific Degree Distribution*. Conference on Uncertainty in Artificial Intelligence (UAI), 2015.
3. Qingming Tang, Jian Peng and Jinbo Xu\*. *Exact Hybrid Covariance Thresholding for Joint Graphical Lasso*. ECML (European Conference on Machine Learning), 2015
4. Siqi Sun and Jinbo Xu\*. *Inferring Block Structure of Graphical Models in Exponential Families*. AI and Statistics (AISTATS) 2015.
5. Jianzhu Ma, Sheng Wang, Zhiyong Wang and **Jinbo Xu\***. *Protein contact prediction by integrating joint evolutionary coupling analysis and supervised learning*. RECOMB2015.
6. Zhiyong Wang, **Jinbo Xu\*** and Xinghua Shi. *CNVnet: Combining Sparse Learning and Biological Networks to Capture Joint Effect of Copy Number Variant*. ACM-BCB 2014. (ACM SIGBio best student paper award)

7. Jianzhu Ma, Sheng Wang and **Jinbo Xu\***. *MRAlign: protein remote homology detection through alignment of Markov Random Fields*. RECOMB2014. (**Best paper award**, also appear at PLOS Computational Biology)
8. Siqi Sun and **Jinbo Xu\***. *Learning block-structured Gaussian Graphical Models via nonparametric method*. AI and Statistics (AISTATS) 2014.
9. Fan Yang, **Jinbo Xu** and Jianyang Zeng. *Drug-target interaction prediction by integrating chemical, genomic, functional and pharmacological data*. Pacific Symposium on Biocomputing (PSB). January 3-7, 2014.
10. Zhiyong Wang, **Jinbo Xu\*** and Xinghua Shi. *Finding alternative eQTLs by exploring sparse model space*. In Proceedings of the RECOMB/ISCB Conference on Regulatory and Systems Genomics, with DREAM Challenges (RECOMB/ISCB RegSys 2013), Toronto, Canada, November 2013.
11. Zhiyong Wang and **Jinbo Xu\***. *Predicting protein contact map using evolutionary and physical constraints by integer programming*. ISMB2013, also appears in *Bioinformatics* (2013) 29 (13):i266-i273.
12. Jianzhu Ma, Sheng Wang, Feng Zhao and **Jinbo Xu\***. *Protein threading using context-specific alignment potential*. ISMB2013, also appears in *Bioinformatics* (2013) 29 (13):i257-i265.
13. Jianzhu Ma, Jian Peng, Sheng Wang and **Jinbo Xu\***. *Estimating the partition function of graphical models using Langevin importance sampling*. AI and Statistics (AISTATS) 2013.
14. Jianzhu Ma, Jian Peng, Sheng Wang and **Jinbo Xu\***. *A conditional neural fields model for protein threading*. ISMB2012, also appears in *Bioinformatics* (2012) 28 (12):i59-i66.
15. Xiaohui Chen, Xinghua Shi, Zhiyong Wang, Xing Xu and **Jinbo Xu\***. *A Two-Graph Guided Multi-task Lasso Approach for eQTL Mapping*. AI and Statistics (AISTATS) 2012.
16. Jian Peng, Nathan Srebro, Tamir Hazan and **Jinbo Xu**. *Approximate Inference with Intersected Outer Bounds and Rounding Schemes*. AI and Statistics (AISTATS), 2012.
17. Zhiyong Wang and **Jinbo Xu\***. *A Conditional Random Fields method for RNA sequence-structure relationship modeling and conformation sampling*. ISMB2011, also appears in *Bioinformatics* (2011) 27 (13):i102-i110.
18. Feng Zhao, Jian Peng and **Jinbo Xu\***. *Fragment-free approach to protein folding using conditional neural fields*. ISMB2010, also appears in *Bioinformatics* (2010) 26 (12):i310-i317.
19. Jian Peng and **Jinbo Xu\***. *Low-homology protein threading*. ISMB2010, also appears in *Bioinformatics* (2010) 26 (12):i294-i300.
20. Jian Peng, Liefeng Bo and **Jinbo Xu**. *Conditional Neural Fields*. NIPS 2009.
21. 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. (**This paper also won the best poster award**)

22. 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.
23. Shuaicheng Li, Dongbo Bu, Xin Gao, **Jinbo Xu\*** and Ming Li. *Designing protein structural alphabets*. ISMB2008, also appears at Bioinformatics (2008) 24 (13):i182-i189.
24. 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, 2008.
25. 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, authors ranked alphabetically**)
26. Rohit Singh, **Jinbo Xu** and Bonnie Berger. *Global Alignment of Multiple Protein Interaction Networks*. In the Proceedings of Pacific Symposium in Biocomputing (PSB) 13:303-314, 2008. Hawaii, USA.
27. **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**)
28. 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**)
29. Xin Gao, Dongbo Bu, ShuaiCheng Li, Ming Li, and **Jinbo Xu\***. *Consensus Contact Prediction by Linear Programming*. Life Science Society Computational Systems Conference (CSB), August 2007. Stanford, USA.
30. 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.
31. 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, 2007.
32. 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.
33. **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.

34. Rohit Singh, **Jinbo Xu** and Bonnie Berger. *Struct2Net: Integrating Structure into Protein-Protein Interaction Prediction*. Pacific Symposium on Biocomputing (PSB) 2006:403-414, Hawaii, USA.
35. **Jinbo Xu**, Feng Jiao and Bonnie Berger. *A Tree-Decomposition Approach to Protein Structure Prediction*. Computational Systems Bioinformatics (CSB), 2005. Stanford, USA.
36. **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. (**An extended version invited to the Journal of the ACM.**)
37. **Jinbo Xu**, Libo Yu and Ming Li. *Consensus Fold Recognition by Predicted Model Quality*. Asia-Pacific Bioinformatics Conference (APBC) 2005:73-83, Singapore.
38. Thomas Tang, **Jinbo Xu** and Ming Li. *Discovery of Sequence-Structure Motifs from Protein Segments and Two Applications*. Pacific Symposium on Biocomputing (PSB) 2005. Hawaii, USA.
39. **Jinbo Xu**, Daniel Brown, Ming Li and Bin Ma. *Optimizing multiple spaced seeds for homology search*. Combinatorial Pattern Matching (CPM) 2004, Istanbul, Turkey.
40. **Jinbo Xu**, Ying Xu, Guohui Lin, Dongsup Kim and Ming Li. *Protein Structure Prediction by Linear Programming*. Pacific Symposium on Biocomputing (PSB) 2003: 264-275, Hawaii, USA.
41. **Jinbo Xu**. *Speed up LP Approach to Protein Threading via Graph Reduction*. in the Proceedings of the 3<sup>rd</sup> International Workshop on Algorithms in Bioinformatics (WABI), Lecture Notes in Computer Science Vol. 2812, pp. 374-388, 2003.

***Peer-reviewed journal papers*** (\* indicates corresponding author)

42. Bingqing Xie, Gady Agam, Sandhya Balasubramanian, **Jinbo Xu**, Conrad Gilliam, Natalia Maltsev, and Daniela Börnigen. *Disease gene prioritization using network and feature information*. Accepted by Journal of Computational Biology, 2015. (also appears at RECOMB Conference on Regulatory and Systems Genomics, with Dream Challenges 2014).
43. Somaye Hashemifar and **Jinbo Xu**\*. *HubAlign: an accurate and efficient method for global alignment of protein-protein interaction networks*. Bioinformatics, 30(17), pp. i438-i444, September 2014.
44. Inna Dubchak, Sandhya Balasubramanian, Sheng Wang, Cem Meyden, Dinanath Sulakhe, Alexander Poliakov, Daniela Börnigen, Bingqing Xie, Andrew Taylor, Jianzhu Ma, Alex R Paciorkowski, Ghayda M Mirzaa, Paul Dave, Gady Agam, **Jinbo Xu**, Lihadh Al-Gazali, Christopher E Mason, M Elizabeth Ross, Natalia Maltsev, T Conrad Gilliam. *An Integrative Computational Approach for Prioritization of Genomic Variants*. PLOS ONE, 2014 Dec 15.
45. Dinanath Sulakhe, Sandhya Balasubramanian, BingqingXie, Bo Feng, Andrew Taylor, Sheng Wang, Eduardo Berrocal, Paul Dave, **Jinbo Xu**, Daniela Bornigen,

- Conrad Gilliam and Natalia Maltsev. *Lynx: a database and knowledge extraction engine for integrative medicine*. Nucleic Acids Research, 2013 Nov 21.
46. Sheng Wang, Jian Peng, Jianzhu Ma and **Jinbo Xu\***. *Protein structure alignment beyond spatial proximity*. (Nature Publishing Group) Scientific Reports, 2013; 3:1448.
  47. Raghavendra Hosur, Jian Peng, Arunachalam Vinayagam, Ulrich Stelzl, **Jinbo Xu**, Norbert Perrimon, Jadwiga Bienkowska and Bonnie Berger. *Coev2Net: a computational framework for boosting confidence in high-throughput protein-protein interaction dataset*. Genome Biology 2012, **13**:R76.
  48. Feng Zhao and **Jinbo Xu\***. *A position-specific distance dependent statistical potential for protein structure and functional study*. (Cell) STRUCTURE, Volume 20, Issue 6, 1118-1126, 17 May 2012.
  49. Morten Kallerg, Haipeng Wang, Jian Peng, Sheng Wang, Zhiyong Wang, Hui Lu and **Jinbo Xu\***. *Template-based protein modeling using the RaptorX web server*. Nature Protocols, 2012 Jul 19; 7(8):1511-22.
  50. Jian Peng and **Jinbo Xu\***. *A multiple-template approach to protein threading*. PROTEINS, Volume 79, Issue 6, pages 1930–1939, June 2011.
  51. Jian Peng and **Jinbo Xu\***. *RaptorX: exploiting structure information for protein alignment by statistical inference*. PROTEINS, Volume 79, Issue S10, pages 161–171, 2011 (**invited paper to CASP9**).
  52. Sheng Wang, Jian Peng and **Jinbo Xu\***. *Alignment of distantly-related protein structures: algorithm, bound and implications to homology modeling*. Bioinformatics, 2011 Sep 15;27(18):2537-45.
  53. 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, 2011 Feb 4; 405(5):1295-310.
  54. 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*. Nucleic acids research, Vol. 38, No. Web Server issue. (July 2010), pp. W508-15. (**The first three authors equally contribute to this paper.**)
  55. 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.
  56. Zhiyong Wang, Jian Peng, Feng Zhao and **Jinbo Xu\***. *Protein 8-class secondary structure prediction using Conditional Neural Fields*. Proteomics, 2011 Oct; 11(19):3786-92. Early version appears in the Proceedings of IEEE BIBM 2010.
  57. Xin Gao, Dongbo Bu, **Jinbo Xu** and Ming Li. *Improving consensus contact prediction via server correlation reduction*. BMC Structural Biology 2009, 9:28
  58. **Jinbo Xu\***, Jian Peng and Feng Zhao. *Template-based and free modeling by RAPTOR++ in CASP8*. PROTEINS, 2009; 77(Suppl 9): 133–137. (**invited paper**)
  59. 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.



60. Feng Zhao, ShuaiCheng Li, Beckett W. Sterner and **Jinbo Xu\***. *Discriminative learning for protein conformation sampling*. PROTEINS, 2008 Oct; 73(1):228-40.
61. Rohit Singh, **Jinbo Xu** and Bonnie Berger. *Global Alignment of Multiple Protein-Protein Interaction Networks*. PNAS, 2008 Sep 2;105(35):12763-8.
62. 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.
63. **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.
64. **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**)
65. **Jinbo Xu\*** and Ming Li. *Assessment of RAPTOR's linear programming approach in CAFASP3*. PROTEINS 2003, 53 Suppl 6:579-84. (**invited paper**)
66. **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.**)
67. **Jinbo Xu**. *Protein Fold Recognition by Predicted Alignment Accuracy*. IEEE/ACM Trans. on Computational Biology and Bioinformatics. 2(2):157-165, 2005.
68. **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.
69. 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 or refereed book chapters***

70. Dinanath Sulakhe, Sandhya Balasubramanian, Bingqing Xie, Eduardo Berrocal, Bo Feng, Andrew Taylor, Bhadrachalam Chitturi, Utpal Dave, Gady Agam, **Jinbo Xu**, Daniela Börnigen, Inna Dubchak, T. Conrad Gilliam, Natalia Maltsev. *High-Throughput Translational Medicine: Challenges and Solutions*. In Systems Analysis of Human Multigene Disorders Advances in Experimental Medicine and Biology Volume 799, 2014, pp 39-67.
71. Morten Källberg, Gohar Margaryan, Sheng Wang, Jianzhu Ma and **Jinbo Xu\***. *RaptorX Server: A Resource for Template-based Protein Structure Modeling*. Methods in Molecular Biology 2013.
72. **Jinbo Xu\***, Libo Yu and Feng Jiao. *Protein Structure Prediction Using Threading*. Book Chapter in Protein Structure Prediction: Methods and Protocols, Humana Press, 2007.
73. Dongbo Bu, Shuaicheng Li, Xin Gao, Libo Yu, **Jinbo Xu** and Ming Li. *Consensus Approaches to Protein Structure Prediction*. In Machine Learning in Bioinformatics, Eds: Yan-Qing Zhang and Jagath C. Rajapakse, John Wiley & Sons, 2007.

## **Books**

74. Jinbo Xu, Jianzhu Ma and Sheng Wang. *Protein Homology Detection Through Alignment of Markov Random Fields*. Springer, 2015.

## **Invited Talks**

Note: this list does not include oral presentations for accepted conference papers.

1. Protein contact prediction by integrating evolutionary and physical constraints. CASP11, December 2014.
2. A context-specific statistical potential empowered by high throughput sequencing. The 2<sup>nd</sup> Zing conferences for protein and RNA structure. December 2013.
3. A new method for de novo transcript assembler. ISMB HitSeq, July 2013. (HitSeq is an ISMB satellite meeting. It does not accept any regular papers, but selects abstracts for oral presentation).
4. Statistical machine learning for protein structure prediction. Arizona State University, April 2013.
5. Statistical machine learning for protein structure prediction. NSF EPSCoR Bioinformatics Workshop to Foster Collaborative Research, March 2013 (**keynote talk**).
6. Protein structure alignment beyond spatial proximity. ISMB2012-3DSIG. (3DSIG is an ISMB satellite meeting. It does not accept any regular papers, but selects abstracts for oral presentation).
7. A context-specific alignment potential for protein threading. CASP10, December 2012 (invited talk)
8. A probabilistic graphical model for protein template-free modeling. CASP10, December 2012 (invited short talk)
9. A context-specific statistical potential for protein structure and functional study. ACM-BCB, October 2012. (invited talk)
10. One invited talk at the 2011 Zing conferences for protein and RNA structure.
11. Statistical learning machines for protein alignment and folding. U Chicago Statistics Department, March 2011.
12. Probabilistic models for protein sequence/structure alignment with application to protein modeling. MIT, Feb 2011.
13. Probabilistic models for protein sequence/structure alignment with application to protein modeling. CMU, Feb 2011.
14. Probabilistic models for protein sequence/structure alignment with application to protein modeling. McGill University, Feb 2011.
15. Three invited talks (2 regular and 1 short) at the CASP9 (the 9<sup>th</sup> Critical Assessment of Structure Prediction) meeting. December, 2010.
16. Probabilistic graphical models for protein structure prediction. Dartmouth College, April 2010.
17. Optimization techniques for protein structure prediction. The Institute of Illinois Technology, March 2010.

18. Protein threading by nonlinearly combining evolutionary and non-evolutionary information. The University of Minnesota, 2009.
19. Protein threading by nonlinearly combining evolutionary and non-evolutionary information. MIT, 2009.
20. Linear programming approach to protein structure prediction. INFORMS Annual Meeting, October 2008.
21. Graph Algorithms for Biological Systems Analysis. SIAM on Discrete Mathematics, June 2008.
22. Global Alignment of Multiple Protein Interaction Networks. The University of Illinois at Chicago, 2008.
23. Protein Conformation Sampling Using Conditional Random Fields, MIT, 2008.
24. Graph Algorithms for Protein Structure Alignment. The 46th IEEE Conference on Decision and Control, December 2007.
25. Knowledge-based Protein Structure Prediction. Institute of Computing Technology, Chinese Academy of Sciences, March 2007. (Distinguished Lecture)
26. Knowledge-based Protein Structure Prediction. Tsinghua University, March 2007.
27. Knowledge-based Protein Structure Prediction. Microsoft Research in Asia, March 2007.
28. Knowledge-based Protein Structure Prediction. Toyota Technological Institute at Japan, April 2007.
29. Protein Side Chain Packing via Tree Decomposition. University of Waterloo, August 2006.
30. A Parameterized Algorithm for Protein Structure Alignment. University of Waterloo, July 2006.
31. A Parameterized Algorithm for Protein Structure Alignment. MIT, May 2006.
32. Knowledge-based Protein Structure Prediction. Northwestern University, May 2006.
33. A Parameterized Algorithm for Protein Structure Alignment. University of Illinois at Chicago, November 2005.
34. Fast and Accurate Algorithms for Protein Side-Chain Packing. Boston University, October 2005.
35. Rapid Protein Side-Chain Packing via Tree Decomposition. DIMACS Workshop on Information Processing by Protein Structures in Molecular Recognition. June 13-14, 2005.
36. RAPTOR: protein threading by linear programming. SIAM mini-symposium, SIAM Conference on Control and Its Applications. New Orleans, LA, July 11-14, 2005.
37. ACE: consensus method to fold recognition. CASP6, Italy. December 2004. (an invitation to our ACE group)
38. Protein Structure Prediction by Linear Programming. School of Medicine, University of Western Ontario, 2004.
39. Protein Structure Prediction. The Interdisciplinary Coffee Talk Society, University of Waterloo, 2003.

## Software, Databases and Servers

1. RaptorX Server for protein structure and function prediction at <http://raptorx.uchicago.edu>. It is one of the three most popular protein structure prediction servers, on average serving **700-800 jobs per week** submitted from around the world. So far RaptorX has more than **12,000 worldwide users**.
2. Standalone protein threading, secondary structure prediction and contact prediction programs are available at <http://raptorx.uchicago.edu/download/>
3. A machine learning tool Conditional Neural Fields: <https://code.google.com/p/cnf/>
4. Struct2Net: a structure-based protein interaction database: <http://groups.csail.mit.edu/cb/struct2net/webserver/>
5. Lynx: a database and knowledge extraction engine for integrative medicine: <http://lynx.ci.uchicago.edu/>
6. Other bioinformatics software developed in my group: <http://ttic.uchicago.edu/~jinbo/software.htm>

## References available on request