Xia Ning

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Research Interests

Xia Ning's research interests focus on Chemoinformatics, Machine Learning and Data Mining (Recommender Systems, Text Mining), and High-Performance Computing. She developed efficient computational algorithms to solve prediction problems for drug discovery purposes (e.g., improved Structure-Activity-Relationship (SAR) models and improved Structure-Activity-Relationship (SSR) models). She also worked on novel machine learning methods (e.g., multi-task learning algorithms, graph kernels) for recommender systems and natural language processing. In addition, she is interested in identifying and solving new learning problems that exist across multiple application domains.

Education

Computer Science & Engineering, University of Minnesota, Twin Cities, Minneapolis, MN, USA

- Ph.D, Computer Science & Engineering — Sept. 2005 – May 2012(anticipated)
  - Adviser: Prof. George Karypis
- M.S., Computer Science & Engineering — Sept. 2005 – Apr. 2009
- M.S., minor, Statistics — Sept. 2005 – Apr. 2009

Chu Kochen Honors College, Zhejiang University, Hangzhou, China

- B.S., Computer Science, with honors — Sept. 2001 – Jun. 2005
  - Adviser: Prof. Yao Zheng

Publications

Journal Papers

[1] X. Ning and G. Karypis, "Improved machine learning models for predicting selective compounds." in preparation for submission to Journal of Chemical Information and Modelling, 2011.

[2] X. Ning and G. Karypis, "In silico structure-activity-relationship (sar) models from machine learning: a review," *Drug Development Research*, 2010.

[3] X. Ning and G. Karypis, "Multi-task learning for recommender systems," in *Journal of Machine Learning Research Workshop and Conference Proceedings*, vol. 13, pp. 269–284, Microtome Publishing, 2010.

[4] X. Ning, H. Rangwala, and G. Karypis, "Multi-assay-based structure-activity-relationship models: Improving structure-activity-relationship models by incorporating activity information from related targets," *Journal of Chemical Information and Modeling*, vol. 49, no. 11, pp. 2444–2456, 2009. PMID: 19842624.

Book Chapter

[5] N. Wale, X. Ning, and G. Karypis, "Trends in chemical graph data mining," in *Managing and Mining Graph Data* (A. K. Elmagarmid, C. C. Aggarwal, and H. Wang, eds.), vol. 40 of *Advances in Database Systems*, pp. 581–606, Springer US, 2010.

Conference Papers

[6] X. Ning and G. Karypis, "Improved machine learning models for predicting selective compounds." ACM Conference on Bioinformatics, Computational Biology and Biomedicine, 2011.

[7] X. Ning and Y. Qi, "Semi-supervised convolution graph kernels for relation extraction," in *SIAM International Conference on Data Mining*, 2011.

[8] X. Ning and G. Karypis, "l_1 induced item similarity matrix for top-n recommendation." submitted to European Conference on Machine Learning and Principle, and Practice of Knowledge Discovery in Databases, 2011.

[9] P. Kuksa, Y. Qi, B. Bai, R. Collobert, J. Weston, V. Pavlovic, and X. Ning, "Semi-supervised abstraction-augmented string kernel for multi-level bio-relation extraction," in *Proceedings of the 2010 European conference on Machine learning and knowledge discovery in databases: Part II*, (Berlin, Heidelberg), pp. 128–144, Springer-Verlag, 2010.

[10] X. Ning and G. Karypis, "The set classification problem and solution methods," in *SIAM International Conference on Data Mining*, pp. 847–858, SIAM, 2009.

[11] J. Chen, Y. Zheng, and X. Ning, "Scalable parallel quadrilateral mesh generation coupled with mesh partitioning," *International Conference on Parallel and Distributed Computing Applications and Technologies*, pp. 966–970, 2005.

Workshop Paper

[12] X. Ning and G. Karypis, "The set classification problem and solution methods," in *IEEE International Conference on Data Mining Workshops*, pp. 720–729, 2008.

Technical Report

[13] X. Ning, H. Rangwala, and G. Karypis, "Improved sar models - exploiting the target-ligand relationships," tech. rep., Computer Science & Engineering, University of Minnesota, 2008.

Talk

[14] X. Ning and G. Karypis, "Evaluation of 3d descriptors in virtual screening." Oral presentation, ACS annual meeting, Sept. 2007.

Patents

Applications

- Systems and methods for semi-supervised relationship extraction, with Y. Qi, P. Kuksa and B. Bai 2011
- Object recognition system with database pruning and querying, with P. Baheti, A. Swaminathan and S. Diaz. 2010

Awards & Honors

Competitions

- Third Prize, the Competition of Mathematical Modeling, Zhejiang, China. 2005
- First Prize, the National Olympic Competition of Physics (**finalist, nationwide top 120**), China. 2001
- First Prize, the National Olympic Competition of Mathematics, China. 1998
- First Prize, the National Olympic Competition of Chemistry, China. 1998

Scholarships

- Departmental nominee, Grad School Doctoral Dissertation Fellowship, University of Minnesota, 2011
- Roberto Patine Scholarship, Qualcomm CR&D, US. 2009
- The Student Innovation Award, Zhejiang University, China. 2005
- The Outstanding Student Award, Zhejiang University, China. 2001 – 2005

Others

- Scholarly Travel Grant, Graduate and Professional Student Assembly, University of Minnesota. 2011
- Travel Award, SIAM International Conference on Data Mining, 2009, 2011
- Travel Award, IEEE International Conference on Data Mining. 2008
- Travel Grant, Office for University Women, University of Minnesota. 2007

Professional Activities

Journal Reviewers

- Bioinformatics, Chemoinformatics, IEEE Transactions on Broadcasting, IEEE Transactions on Knowledge and Data Engineering, IEEE The Journal of Selected Topics in Signal Processing, International Journal of Pattern Recognition, Journal of Chemical Information and Modeling, Journal of Zhejiang University-SCIENCE A

Conference Reviewers

- BIBE, CIKM, ECML/PKDD, GIW, ICCABS, ICDM, IPDPS, ISBRA, KDD, KDIR, MLG, PAA, PAKDD, SDM

Research Experience

Graduate Research Assistant Jun. 2006 – now

- Chemoinformatics, Machine Learning, Data Mining, Karypis Lab, Jan. 2007 - now
  - Compound binding conformation detection
  - Compound activity prediction
  - Structure-Activity-Relationship (SAR) model improvement
  - Structure-Selectivity-Relationship (SSR) model improvement
  - Set classification
  - Multi-task learning for collaborative filtering
  - l_1 minimization for top-n recommendation
- Computational Geometry Jun. 2006 – Dec. 2006
  - Geometric algorithm for rapid prototyping, with Prof. Ravi Jarnadan

Undergraduate Research Assistant Sept. 2004 – Jun. 2005

- Mesh generation, Center for Engineering and Scientific Computation, Zhejiang University, China
  - Mesh generation algorithms and graph partitioning algorithms
  - Undergrad thesis

Teaching Experience

Graduate Teaching Assistant Sept. 2005 – Dec. 2006

- CSCI4041, Algorithms and Data Structures, undergrad level
- CSCI5421, Advanced Algorithms and Data Structures, grad level
- CSCI5481, Computational Genomics, grad level
- Assignment and exam grading, TA office hours and recitation sessions

Undergraduate Teaching Assistant Sept. 2002 – Jun. 2003

- Mathematical Analysis
  - Advanced mathematics course for outstanding freshmen students

- Graduate teaching assistant appointment assigned to sophomores (**7 out of 10,000** undergrads)

- Assignment and exam grading, recitation sessions

Professional Experience

Machine Learning Department, NEC Labs America, NJ

- Summer Research Assistant — Jun. 2010 – Sept. 2010
  - Text mining for Bio-relation extraction

Corp R&D, Qualcomm, CA

- Engineering Interim Intern — Jun. 2009 – Sept. 2009, Jul. 2008 – Sept. 2008
  - Data mining algorithm design and implementation for Augmented Reality
  - Parallel clustering algorithm implementation