# BIOKDD04: Workshop on Data Mining in Bioinformatics August 22nd, 2004 Seattle, WA, USA

in conjunction with

10th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining

Mohammed J. Zaki Computer Science Department Rensselaer Polytechnic Institute Troy, NY 12180, USA zaki@cs.rpi.edu

Shinichi Morishita
Department of Computational
Biology
University of Tokyo
Kashiwa City, Chiba, Japan
moris@k.u-tokyo.ac.jp

Isidore Rigoutsos, PhD Manager, Bioinformatics & Pattern Discovery Group IBM Thomas J Watson Research Center Yorktown Heights, NY 10598 rigoutso@us.ibm.com

#### **Opening Remarks**

Bioinformatics is the science of managing, mining, and interpreting information from biological sequences and structures. Genome sequencing projects have contributed to an exponential growth in complete and partial sequence databases. The structural genomics initiative aims to catalog the structure-function information for proteins. Advances in technology such as microarrays have launched the subfield of genomics and proteomics to study the genes, proteins, and the regulatory gene expression circuitry inside the cell. What characterizes the state of the field is the flood of data that exists today or that is anticipated in the future; data that needs to be mined to help unlock the secrets of the cell.

While tremendous progress has been made over the years, many of the fundamental problems in bioinformatics, such as protein structure prediction or gene finding, are still open. Data mining will play a fundamental role in understanding gene expression, drug design and other emerging problems in genomics and proteomics. Furthermore, text mining will be fundamental in extracting knowledge from the growing literature in bioinformatics.

The goal of this workshop is to encourage KDD researchers to take on the numerous challenges that Bioinformatics offers. The workshop features an invited talks from noted expert in the field, and the latest data mining research in bioinformatics. We encouraged papers that propose novel data mining techniques for tasks such as:

- $\bullet$  Gene expression analysis
- Protein/RNA structure prediction
- ullet Phylogenetics
- Sequence and structural motifs
- Genomics and Proteomics
- Gene finding
- Drug design
- RNAi and microRNA Analysis
- Text mining in bioinformatics
- Modeling of biochemical pathways

These proceedings contain 10 papers (6 long and 4 short), out of 26 submissions that were accepted for presentation at the workshop. Each paper was reviewed by three members of the program committee. Along with a keynote talk, we were able to assemble a very exciting program.

We would like to thank all the authors, invited speaker, and attendees for contributing to the success of the workshop. Special thanks are due to the program committee for help in reviewing the submissions.

This workshop follows the previous three highly successful workshops: BIOKDD03, held in Washington, DC; BIOKDD02, held in Edmonton, Canada; and BIOKDD01 held in San Francisco, CA. We expect BIOKDD04 to be equally successful.

## **Workshop Co-Chairs**

- Mohammed J. Zaki, Rensselaer Polytechnic Institute
- Shinichi Morishita, University of Tokyo
- Isidore Rigoutsos, IBM T.J. Watson Research Center

#### **Program Committee**

• Srinivas Aluru, Iowa State U., USA • Alberto Apostolico, Prudue U., USA • Tatsuya Akutsu, Kyoto U., Japan • Charles Elkan, UC San Diego, USA • Jayant Haritsa, Indian Inst. of Science, India • Hasan Jamil, Wayne State U., USA • Andreas Karwath, U. Freiburg, Germany • George Karypis, U. Minnesota, USA • Ross D. King, U. of Wales, UK • Jinyan Li, Inst. for Infocomm Research, Singapore • Lance A. Liotta, NIH/NCI, USA • Ambuj Singh, UC Santa Barbara, USA • David Page, U. Wisconsin, USA • Srinivasan Parthasarathy, Ohio State U., USA • Jignesh M. Patel, U. Michigan, USA • Daniel E. Platt, IBM TJ Watson, USA • Luc De Raedt, U. Freiburg, Germany • Tobias Scheffer, Humboldt U., Germany • Karlton Sequeira, RPI, USA • Hannu Toivonen, U. Helsinki, Finland • Jason Wang, NJIT, USA • Wei Wang, UNC Chapel-hill, USA • Jiong Yang, Case Western Reserve U., USA • Aidong Zhang, U. Buffalo, USA

### **Workshop Program & Table of Contents**

8:50-9:00am: Opening Remarks

9:00-10:00am: Session I

- 9:00-9:30 (long) A New Approach to Protein Structure Mining and Alignment, Hongyuan Li, Keith Marsolo, Srinivasan Parthasarathy, Dmitrii Polshakov, The Ohio State University page 1
- 9:30-10:00 (long) A Novel Approach for Prediction of Protein Subcellular Localization from Sequence Using Fourier Analysis and Support Vector Machines, Zhengdeng Lei, Yang Dai, Univ. of Illinois at Chicago page 11

10:00-10:30am: Coffee Break 10:30-11:15am: Keynote Talk

Mark Boguski, M.D, Ph.D., Senior Director, Development and Research, Allen Institute for Brain Science; and affiliate
faculty, Fred Hutchinson Cancer Research Center & Department of Medicine/Genetics, University of Washington.

#### 11:15-11:55am: Session II

- 11:15-11:35 (short) High-throughput Protein Interactome Data: Minable or Not? Jake Chen, Andrey Sivachenko, Lang Li, Indiana University page 18
- 11:35-11:55 (short) Assessment of discretization techniques for relevant pattern discovery from gene expression data, Ruggero Pensa, Claire Leschi, Jeremy Besson, Jean-Francois Boulicaut, INSA, Lyon (France) page 24

12:00-1:30pm: Lunch 1:30-3:00pm: Session III

- 1:30-2:00 (long) Meta-classification of Multi-type Cancer Gene Expression Data, Benny Yin-ming Fung, Vincent To-yee Ng, Hong Kong Polytechnic University page 31
- 2:00-2:30 (long) Bayesian Model-Averaging in Unsupervised Learning From Microarray Data, Mario Medvedovic, Junhai Guo, University of Cincinnati page 40
- 2:30-2:50 (short) Clustering Labeled Data and Cross-Validation for Classification with Few Positives in Yeast, Miles Trochesset, Anthony Bonner, Univ. of Toronto page 48
- 2:50-3:10 (short) A Maximum Entropy Approach to Biomedical Named Entity Recognition, Yi-Feng Lin, Tzong-Han Tsai, Wen-Chi Chou, Kuen-Pin Wu, Ting-Yi Sung, Wen-Lian Hsu, IIS, Academia page 56

3:10-3:30pm: Coffee Break 3:30-4:30pm: Session IV

- 3:30-4:00 (long) Discovering Spatial Relationships Between Approximately Equivalent Patterns in Contact Maps, Keith Marsolo, Hui Yang, Srinivasan Parthasarathy, Sameep Mehtas, The Ohio State University
   page 62
- 4:00-4:30 (long) Differential Association Rule Mining for the Study of Protein-Protein Interaction Networks, Christopher Besemann, Anne Denton, Ajay Yekkirala, Ron Hutchison, Marc Anderson, North Dakota State University page 72