24th International Conference on Genome Informatics (GIW2013)

16 – 18 December 2013
Matrix, Biopolis, Singapore

Welcome

We warmly welcome you to the 24th International Conference on Genome Informatics (GIW 2013) at the Biopolis in Singapore on 16-18 December 2013. The GIW is the longest running international bioinformatics conference. The aims of the conference are to present recent results of both theoretical and practical research, to show new applications, to demonstrate systems, and to indicate directions of future research. We cordially invite you to participate. The conference features 3 keynote talks, 7 other invited talks, and over 40 presentations of contributed papers, as well as 2 poster sessions. This booklet provides you some briefly relevant information on the conference.

Acknowledgements

We thank the participants for the very large number of paper submissions and the programme committee members for their hard work under the tight reviewing deadline. We also appreciate the strong and generous support from the National University of Singapore, the BioInformatics Institute, the Genome Institute of Singapore, and the Institute for Infocomm Research.

Limsoon Wong (Conference Chair)
Frank Eisenhaber (PC Co-Chair)
Wing-Kin Sung (PC Co-Chair)

Conference Programme

Day 1: 16 December 2013, Monday

8.30am – 9.15am @ Matrix Level 4 Foyer
Breakfast

9.15am – 9.30am @ Exploration Theatrette
Opening Messages

Limsoon Wong, Frank Eisenhaber & Wing-Kin Sung

9.30am – 10.20am @ Exploration Theatrette.
Keynote 1. Chair: Wing-Kin Sung

William S. Noble, University of Washington: "The one-dimensional and three-dimensional structure of the genome"

10.30am – 11.30am @ Exploration Theatrette.
Session 1.1A: Motif. Chair: Wing-Kin Sung

41. Tzu-Hsien Yang and Wei-Sheng Wu: "Inferring functional transcription factor-gene binding pairs by integrating transcription factor binding data with transcription factor knockout data"

71. Agnieszka Podsiadlo, Mariusz Wrzesien, Wieslaw Paja, Witold Rudnicki and Bartek Wilczynski: "Active enhancer activity can be accurately predicted from chromatin marks and collective sequence motif data"

53. Yanglan Gan, Jihong Guan, Shuigeng Zhou and Weixiong Zhang: "Identifying cis-regulatory elements and modules using conditional random fields"

10.30am – 11.30am @ Creation Theatrette
Session 1.1B: Microarray & Phage Display.
Chair: Vladimir Kuznetsov

61. Chia-Chun Chiu, Shih-Yao Chan, Chung-Ching Wang and Wei-Sheng Wu: "Missing value imputation for microarray data: A comprehensive comparison study and a web tool"

46. Hsiuying Wang, Chia-Chun Chiu, Yi-Ching Wu and Wei-Sheng Wu: "Shrinkage regression-based methods for microarray missing value imputation"

43. Beibei Ru, Peter A.C. 't Hoen, Fulei Nie, Hao Lin, Feng-Biao Guo and Jian Huang: "PhD7Faster: Predicting clones propagating faster from the Ph.D.-7 phage display peptide library"

11.30am – 1.30pm @ Matrix Level 4 Foyer
Lunch Break & Poster Session (Even-Numbered Posters)

1.30pm – 2.20pm @ Exploration Theatrette
Invited Talk 1. Chair: Manju Bansal

Sebastian Maurer-Stroh, BioInformatics Institute, A*STAR: "Chasing the next superbug from the safety of our computer"

2.30pm – 3.30pm @ Exploration Theatrette
Session 1.2A: Protein Structure. Chair: Jinyan Li

68. Laleh Soltan Ghoraie, Forbes Burkowski, Shuai Cheng Li and Mu Zhu: "Residue-specific side-chain polymorphisms via particle belief propagation"

14. Ying Fan, Ruoshui Lu, Lusheng Wang, Massimo Andreatta and Shuai Cheng Li: "Quantifying significance of MHC II residues"

29. Paul Yoo, Sami Muhaidat, Kamal Taha, Jamal Bentahar, Abdallah Shami: "Intelligent consensus modeling for proline cis-trans isomerization prediction"

2.30pm – 3.30pm @ Creation Theatrette
Session 1.2B: Biomarkers. Chair: Hideo Matsuda

28. Wan-Shu Cheng and Jung-Hsien Chiang: "CGPredictor: A systematic integrated analytic tool for mining and examining genome-scale cancer independent prognostic epigenetic marker panels"

94. Mani P. Grover, Sara Ballouz, Kaavya Mohanasundaram, R.A. George, Craig Sherman, Tamsyn Crowley and Merridee Wouters: "Identification of novel therapeutics for complex diseases from genome-wide association data"

93. Henry Han, Xiao-Li Li, See-Kiong Ng and Zhou Ji: "Multi-resolution test for consistent phenotype discrimination and biomarker discovery in translational bioinformatics"

3.30pm – 4.00pm @ Matrix Level 4 Foyer
Tea Break

4.00pm – 5.00pm @ Exploration Theatrette
Session 1.3A: Sequencing. Chair: Lusheng Wang

18. Takahiro Mimori, Naoki Nariai, Kaname Kojima, Mamoru Takahashi, Akira Ono, Yukuto Sato, Yumi Yamaguchi-Kabata and Masao Nagasaki: " iSVP: An integrated structural variant calling pipeline from high-throughput sequencing data"

11. Yi-Min Chen, Chun-Hui Yu, Chi-Chuan Hwang and Tsunglin Liu: "OMACC: An Optical-Map-Assisted Contig Connector for improving de novo genome assembly"

33. Ruiqi Liao, Ruichang Zhang, Jihong Guan and Shuigeng Zhou: "A new unsupervised binning approach for metagenomic sequences based on n-grams and automatic feature weighting"

4.00pm – 5.00pm @ Creation Theatrette
Session 1.3B: Translational Medicine. Chair: Xiaoli Li

30. Hiroaki Iwata, Sayaka Mizutani, Yasuo Tabei, Masaaki Kotera, Susumu Goto and Yoshihiro Yamanishi: " Inferring protein domains associated with drug side effects based on drug-target interaction network"

38. Yasuo Tabei and Yoshihiro Yamanishi: "Scalable prediction of compound-protein interactions using minwise hashing"

31. Masaaki Kotera, Yasuo Tabei, Yoshihiro Yamanishi, Yuki Moriya, Toshiaki Tokimatsu, Minoru Kanehisa and Susumu Goto: " KCF-S: KEGG Chemical Function and Substructure for improved interpretability and prediction in chemical bioinformatics"

6.15pm – 8.15pm @ Penang Place
Welcome Reception

Reception venue: Penang Place, 1 Fusionopolis Way, Connexis #B1-20. Tel: +65 6467 7003.

Day2 : 17 December 2013, Tuesday

8.30am – 9.30pm @ Matrix Level 4 Foyer.
Breakfast

9.30am – 10.20am @ Exploration Theatrette
Keynote 2. Chair: Frank Eisenhaber

Manju Bansal, Indian Institute of Science: "Role of DNA sequence and structural features of promoter regions in gene expression in S. cerevisiae"

10.30am – 11.30am @ Exploration Theatrette
Session 2.1A: Phylogenetics. Chair: Wing Cheong Wong

48. Sebastian Maurer-Stroh, Vithiagaran Gunalan, Wing Cheong Wong and Frank Eisenhaber: "A simple shortcut to unsupervised alignment-free phylogenetic genome groupings, even from unassembled sequencing reads"

47. Jianmin Ma, Frank Eisenhaber and Sebastian Maurer-Stroh: "Automatic phylogenetic classification of bacterial beta-lactamase sequences including structural and antibiotic substrate preference information"

5. Jing-Doo Wang: "Comparing virus classification using genomic materials according to different taxonomic levels"

10.30am – 11.30am @ Creation Theatrette
Session 2.1B: Protein-Protein Interactions. Chair: Hiroshi Mamitsuka

9. Slavka Jaromerska, Petr Praus and Young-Rae Cho: "Distance-wise pathway discovery from protein-protein interaction networks weighted by semantic similarity"

56. Chasanah Kusumastuti Widita and Osamu Maruyama: "PPSampler2: Predicting protein complexes more accurately and efficiently by sampling"

73. Florian Goebels and Dmitrij Frishman: "Prediction of protein interaction types based on sequence and network features"

11.30am – 1.30pm @ Matrix Level 4 Foyer
Lunch Break & Poster Session (Odd-Numbered Posters)

1.30pm – 2.20pm @ Exploration Theatrette
Invited Talk 2. Chair: William S. Noble

P. S. Thiagarajan, National University of Singapore: "Analysis of ODE models of bio-pathways using statistical model checking"

2.30pm – 3.30pm @ Exploration Theatrette
Session 2.2A: Phylogenetics. Chair: William S. Noble

84. Sriganesh Srihari, Venkatesh Raman, Hon Wai Leong and Mark Ragan: "Evolution and controllability of cancer networks: A Boolean perspective"

69. Jing Guo, Ritika Jain, Peng Yang, Rui Fan, Chee Keong Kwoh and Jie Zheng: "Reliable and fast estimation of recombination rates by convergence diagnosis and parallel Markov chain Monte Carlo"

76. Yuta Taniguchi, Yasuhiro Yamada, Osamu Maruyama, Satoru Kuhara and Daisuke Ikeda. "The purity measure for genomic regions leads to horizontally transferred genes"

2.30pm – 3.30pm @ Creation Theatrette
Session 2.2B: Text Mining. Chair: See-Kiong Ng

54. Jui-Chen Hsiao, Chih-Hsuan Wei and Hung-Yu Kao: "Gene name disambiguation using multi-scope species detection"

44. Claudiu Mihaila and Sophia Ananiadou: "Recognising discourse causality triggers in the biomedical domain"

39. Oliver Tessmer, Yuhua Jiao, Jeffery A. Cruz, David M. Kramer and Jin Chen: "Functional approach to high-throughput plant growth analysis"

3.30pm – 4.00pm @ Matrix Level 4 Foyer
Tea Break

4.00pm – 5.30pm @ Exploration Theatrette
AASBi Session. Chair: Limsoon Wong

Satoru Miyano, University of Tokyo: "Cancer gene network analysis"

Hiroshi Mamitsuka, Kyoto University: "Efficiently detecting switching mechanisms in gene expression"

Xiaoli Li, Institute for Infocomm Research, A*STAR: "Biological network mining for modules, disease genes, drug-target interactions"

7.00pm – 9.30pm @ The Jewel Box
Conference Banquet

Banquet venue: 109 Mount Faber Road. Tel: +65 6270 8855. http://www.mountfaber.com.sg

18 December 2013, Wednesday

8.30am – 9.30pm @ Matrix Level 4 Foyer.
Breakfast

9.30am – 10.20am @ Exploration Theatrette
Keynote 3. Chair: Frank Eisenhaber

Shamil Sunyaev, Brigham & Women's Hospital: "Computational methods for sequencing studies in Mendelian and complex traits genetics"

10.30am – 11.30am @ Exploration Theatrette
Session 3.1A: Systems Biology. Chair: Pauline Ng

13. Kyung-Ah Sohn, Dokyoon Kim, Jaehyun Lim and Ju Han Kim: "Relative impact of multi-layered genomic data on gene expression phenotypes in serous ovarian tumors"

51. Meiyappan Lakshmanan, Bevan Kai-Sheng Chung, Chengcheng Liu, Seon-Won Kim and Dong-Yup Lee: "Cofactor modification analysis: A computational framework to identify cofactor specificity engineering targets for strain improvement"

52. Jiin Choi and Taesung Park: "Multivariate generalized multifactor dimensionality reduction to detect gene-gene interactions"

11.30am – 1.00pm @ Matrix Level 4 Foyer
Lunch Break

1.00pm – 1.50pm @ Exploration Theatrette
Invited Talk 3. Chair: Shamil Sunyaev

Chiea Chuen Khor, Genome Institute of Singapore, A*STAR: "Genetics of common diseases in Asia. How has Bioinformatics helped us?"

2.00pm – 3.00pm @ Exploration Theatrette
Session 3.2A: Systems Biology. Chair: P. S. Thiagarajan

10. Zhongyuan Tian, Adrien Faure, Hirotada Mori and Hiroshi Matsuno: "Identification of key regulators in glycogen utilization in E. coli based on the simulations from a hybrid functional Petri net model"

65. Masahiko Nakatsui, Michihiro Araki and Akihiko Kondo: "An approach for dynamical network reconstruction of simple network motifs"

1. Hufeng Zhou, Javad Rezaie, Willy Hugo, Shangzhi Gao, Jingjing Jin, Mengyuan Fan, Chern Han Yong, Michal Wozniak and Limsoon Wong, : "Stringent DDI-based prediction of H. sapiens–M. tuberculosis H37Rv protein-protein interactions"

3.00pm – 3.30pm @ Matrix Level 4 Foyer
Tea Break

3.30pm – 4.30pm @ Exploration Theatrette
Session 3.3A: Algorithm and Data-Mining.
Chair: Hon Wai Leong

55. Yu-Lun Chen, Tun-Wen Pai, Chien-Ming Chen, Hon-Wai Leong and Ket-Fah Chong: "Homolgous synteny block detection based on suffix tree algorithms"

32. Yang Zhao, Morihiro Hayashida, Jira Jindalertudomdee, Hiroshi Nagamochi and Tatsuya Akutsu: "Breadth first search approach to enumeration of tree-like chemical compounds"

8. Liang Zhao, Steven C.H. Hoi, Zhenhua Li, Limsoon Wong, Hung Nguyen and Jinyan Li: "Coupling graphs, efficient algorithms and B-cell epitope prediction"

4,30pm – 4.40pm @ Exploration Theatrette
Closing Messages

Limsoon Wong

Keynotes and Invited Talks

Keynotes

Role of DNA sequence and structural features of promoter regions in gene expression in *S. cerevisiae*

Manju Bansal
Indian Institute of Science

Gene expression is a fundamental biological process, in which the genetic information coded in DNA is used to create a phenotype. It can be regulated and modulated at various levels, such as during transcription, RNA processing, translation and post translational events. The initiation of transcription is the first and most important step in regulation of gene expression and promoter regions are the elements where the transcription machinery assembles . So the level of gene expression depends on promoter architecture, along with other external factors. Presence of motifs (TFBSs, TATA-box , etc.) or cytosine methylation in vertebrates are essential for regulation of gene expression in Eukaryotes, but their role in regulation of gene expression is restricted to a few sets of genes. On the other hand, several experimental and computational studies have shown that promoter sequences possess some special properties, such as low stability, less bendability, low nucleosome occupancy and more curvature, which are common across all organisms. These structural features may play a role in regulation of gene expression at transcription level. We have analyzed the relationship between promoter-specific features (motifs, DNA structural features), promoter directionality (uni or bi-directional) and gene expression variability. This relationship has been examined for seven different experimentally reported gene expression variability measures, along with two measures of regulatory effect, for *S. cerevisiae*. We find that several gene expression variability measures are weakly linked to DNA structural properties, nucleosome occupancy, TATA box presence and bi-directionality of promoter regions. Interestingly, one gene expression variability measure, gene responsiveness is found to be intimately correlated to promoter architecture. So, with proper estimate of structural properties of gene promoters, their expression levels can be predicted. Prediction and characterization of gene promoters corresponding to different gene expression levels using our our in-house software 'PromPredict' will be discussed.

Brief bio. Manju Bansal graduated with a degree in Physics from Osmania University, India in 1972. She then joined the Molecular Biophysics Unit, Indian Institute of Science for PhD and obtained her doctoral degree in 1977 on theoretical studies of collagen structure and stability. She did post-doctoral work at IISc and was a von Humboldt Fellow at EMBL, Heidelberg. She has been a faculty member of IISc since 1982. Converting sequence and structural data into useful functional information is one of the major challenges facing modern biology. Professor Manju Bansal has made several important contributions in this field by developing new computational tools and using them for analysis and prediction of biologically relevant features in proteins and nucleic acids. Some of the predictions have been experimentally verified, in collaboration with others. In particular her work on role of hydroxyproline in stabilization of collagen structure, analysis of helical structures in proteins, modeling of triplex and G-quadruplex structures of DNA is well recognized. More recently the work on analysis and identification of structural properties of regulatory regions in non-coding DNA, at whole genome level has provided new insights about promoter regions in bacteria as well as plants. Based on this research, Prof Bansal has published more than 100 papers in peer reviewed journals. In recognition of her expertise in nucleic acid structure analysis and modeling, Prof. Bansal was invited to be member of a committee to define the structural parameters and their nomenclature for nucleic acids. She has also served on the editorial board of several journals and is a member of the International Advisory

Committee of the World Wide Protein Data Bank since 2005.

The one-dimensional and three-dimensional structure of the genome

William S. Noble
University of Washington

A variety of molecular biology technologies have recently made it clear that the function of the genome in vivo is determined both by the linear sequences of nucleotides along the chromosome and the three-dimensional conformation of chromosomes within the nucleus. In this talk, I will describe computational and statistical methods that we have developed and applied to a variety of genomes, with the goal of characterizing genome architecture and function. In particular, we have used unsupervised and semisupervised machine learning methods to infer the linear state structure of the genome, as defined by a large panel of epigenetic data sets generated by the NIH ENCODE Consortium, and we have developed methods to assign statistical confidence and infer the 3D structure of genomes from Hi-C data.

Brief bio. Wiliam Stafford Noble graduated from Stanford University in 1991 with a degree in Symbolic Systems. Between undergraduate and graduate school, he worked in the speech group at SRI International in Menlo Park, CA, and at Entropic Research Laboratory in Palo Alto, CA. He also spent two years teaching high school math, physics and English literature with the US Peace Corps in Lesotho, Africa. In 1994, he entered graduate school at the University of California, San Diego, where he studied with Charles Elkan. He received the Ph.D. in computer science and cognitive science in 1998. He then spent one year as a Sloan/DOE Postdoctoral Fellow with David Haussler at the University of California, Santa Cruz. From 1999 until 2002, Noble was an Assistant Professor in the Department of Computer Science at Columbia University, with a joint appointment at the Columbia Genome Center. In 2002, he joined the faculty of the Department of Genome Sciences at the University of Washington, where he has adjunct appointments in the Department of Computer Science and Engineering and in the Department of Medicine. His research group develops and applies statistical and machine learning techniques for modeling and understanding biological processes at the molecular level. Noble is the recipient of an NSF CAREER award and is a Sloan Research Fellow.

Computational methods for sequencing studies in Mendelian and complex traits genetics

Shamil Sunyaev
Brigham & Women's Hospital

Rapid development of technology propels applications of DNA sequencing in genetics of both Mendelian and complex trait phenotypes. In Mendelian genetics, sequencing of a single parent-child trio frequently provides promising candidate mutations. Known population genetics parameters and experience with real cases suggest that only a few variants usually fit the inheritance pattern under the assumption of complete penetrance. These variants are further prioritized at the gene level based on available genetic data, functional data, data on expression and interactions. At the variant level, we are developing computational methods for predicting functionally significant mutations. Statistical models informed by population genetics provide estimates of the background probability to observe variants fitting the inheritance pattern by chance. Sequencing studies of individual human patients with Mendelian disorders lead to discoveries of new biology. The success of finding causal variants in small samples in Mendelian genetics does not translate to complex trait genetics. The promise of sequencing studies in complex trait genetics is grounded in population genetics and in success of candidate gene sequencing studies. Sequencing studies require a toolkit of statistical methods different from studies of common variants. These methods can be assisted by functional considerations and take into account allele frequency distribution. However, power of sequencing studies focusing on rare variants is low and many current studies are underpowered. A study of Early Onset Myocardial Infarction provides an example of exome-wide significant signals detected in a sequencing study.

Brief bio. Shamil Sunyaev received his PhD from Moscow Insitute of Physics and Technology (MIPT) and completed postdoctoral training at European

Molecular Biology Laboratory (EMBL). He is now an Associate Professor at Genetics Division, Brigham & Women's Hospital, Harvard Medical School. He is also a member of Harvard-M.I.T. Health Sciences and Technology Division. His interests include computational analysis of human genetic variation, comparative genomics and computational proteomics.

Invited Talks

Genetics of common diseases in Asia. How has Bioinformatics helped us?

Chiea Chuen Khor
Genome Institute of Singapore, A*STAR

Genome-wide association studies have revolutionized the study of human heredity over the past 6 years. This is so because previous candidate-gene based genetic studies had severe techological limitations, which in turn limited the perspective in which we could view the context of our experiments. Together with triumphs in microarray design, the succeess of the GWAS approach in identifying robust determnants of disease susceptibiltiy is due mainly in the advances in conceptual Genome Informatics, which allow the analysis to be done in unprecedentedly precise fashion. Compensations and statistical adjustments which were previously thought impossible are now routinely done. I will attempt to share with you our journey in the study of medical genetics, and the road ahead when deep re-sequencing becomes more and more widespread.

Brief bio. Dr Chiea Chuen Khor qualified as a medical doctor, but found science to be his true professional calling. Together with local and overseas clinician partners, he has been responsible for the conduct of genome-wide association studies on Asian-centric diseases such as Kawasaki disease, Dengue shock, Primary angle closure glaucoma, as well as age-related macular degeneration. These findings clearly demonstrate that often, the Asian form of such diseases have distinct genetic architectures compared to Europeans, which explain why these diseases present differently, respond differently, and are even present at different frequency of prevalence in Asians compared to Europeans. He currently leads a research group at the Genome Institute of Singapore, and has been a regular contributor to research published in Nature Genetics, American Journal of Human Genetics, as well as Human Molecular Genetics.

Chasing the next superbug - from the safety of our computer

Sebastian Maurer-Stroh
Bioinformatics Institute, A*STAR

The threat of serious infectious disease outbreaks is real. Even in the last decade alone we saw the deadly SARS, the global pandemic H1N1 influenza, rise of multidrug resistant bacteria, avian influenzas H5N1 and H7N9 and a novel coronavirus causing serious infections in humans. While media attention spurs popularity of the topic, there has also been a revolution in our abilities to detect and follow-up these pathogens through cheaper and faster sequencing technologies. We are literally flooded with sequence data needing interpretation but making biological and medical sense out of the sequences remains a challenge and requires a multidisciplinary approach at the interface of computational algorithms, evolution and medical biology. I will show examples how, from the safety of our computer, we tackle the critical task of going from sequence to structure and function to better understand infectious disease pathogens and their effect on the host.

Brief bio. Sebastian Maurer-Stroh studied theoretical biochemistry at the University of Vienna and wrote his master and PhD thesis at the renowned Institute of Molecular Pathology (IMP). Following the honours of a FEBS and a Marie Curie fellowship at the VIB-SWITCH lab in Brussels, he now leads a group of experts in protein sequence analysis as principal investigator in the A*STAR Bioinformatics Institute (BII) since November 2007. He has contributed widely used predictors for posttranslational lipid modifications, amyloid fibre formation and catalyzed new biomedical insights by sequence-based function predictions. He has been at the forefront of research during the 2009 H1N1 pandemic collaborating with hospitals and health authorities in Singapore, Mexico, Brazil and Australia. He also initiated a cross-division programme for Human Infectious Diseases at the Bioinformatics Institute that builds upon the expertise of several groups from different backgrounds and for which he is programme director since 2010. He is also adjunct

assistant professor at the Nanyang Technological University's School of Biological Sciences and appointed as visiting scientist to the National Public Health Laboratory of the Ministry of Health Singapore.

Analysis of ODEs models of bio-pathways using statistical model checking

P. S. Thiagarajan
National University of Singapore

The dynamics of biochemical networks -- often called bio-pathways – govern a variety of cellular functions. Their malfunctioning can lead to major diseases. Thus it is important to understand their behavior using mathematical models. Ordinary differential equations (ODEs) are a well-established formalism for modeling biochemical networks in which the time evolution of the concentration levels of each molecular species in the network is captured by a differential equation that captures the kinetics of the reactions that this species participates in. In the study of such ODEs systems it is important to take into account cell-to-cell variability in the values of the initial conditions as well as the rate constants that govern the kinetics of the various reactions in the network. We do so by using probability distributions to model a set of initial concentrations and kinetic rate values. We then develop a statistical model checking (SMC) procedure for verifying the dynamical properties of an ODE system accompanied by such prior distributions. In our specification logic both qualitative properties of the pathway and experimental data can be encoded. This enables us to develop SMC based parameter estimation and sensitivity analysis procedures. We have validated our method on large pathway models. We are currently extending this technique to handle multi-mode ODEs models of bio-pathways.

Brief bio. P.S. Thiagarajan is a Professor in the Department of Computer Science, National University of Singapore and a Senior Faculty Member of the NUS Graduate School of Integrative Science and Engineering (NGS). He received a B.Tech (Electronics) degree from the Indian Institute of Technology, Madras, India (1970) and a PhD degree (Computer Science) from Rice University, Houston, Texas, USA (1973). Before coming to NUS his research had been devoted to various aspects of the theory of distributed systems including Petri nets, temporal logics and supervisory control. After moving to NUS, he has focused mainly on real time, hybrid and embedded computing systems. In recent years, his interest has shifted to computational systems biology. He has given invited talks in most of the leading conferences in his areas of research. He is a Fellow of the Indian Academy of Sciences and a Fellow of the Indian National Academy of Sciences and has served on the Governing Council of the European association for Theoretical Computer Science (1997-2003). He is currently a member of the Academic Council of the Chennai Mathematical Institute. He also serves on the editorial boards of The Real-Time Systems journal and Transactions on Petri nets and Other Models of Concurrency.

AASBi Talks

Biological network mining for modules, disease genes, drug-target interactions

Xiaoli Li
Institute for Infocomm Research, A*STAR

In recent years, a number of biological networks, such as protein interaction networks, disease phenotype networks, drug-target networks etc., have become available for detecting novel biological knowledge through biological network mining. Here, I will present the following three network mining research topics, namely, 1) how to identify protein complexes from protein interaction networks; 2) how to detect disease genes by constructing heterogeneous networks, such as protein interaction networks, phenotype networks etc; 3) how to predict novel disease drug-target interactions based on our proposed network mining approach.

Brief bio. Xiaoli Li is currently a machine learning lab head and senior scientist at the Institute for Infocomm Research, A*STAR, Singapore. He also holds an adjunct appointment in the SCE, Nanyang Technological University. His research interests include bioinformatics, data mining, and machine learning. He has been serving as a member of technical program committees in the leading data

mining related conferences (KDD, ICDM, SDM, PKDD/ECML, PAKDD, WWW, AAAI, and CIKM), as well as being the co-Editor-in-Chief of International Journal of Knowledge Discovery in Bioinformatics (IJKDB). His highly-cited research include positive unlabelled learning, biological/social network mining, etc. In 2005, he received the Best Paper Award in the 16th International Conference on Genome Informatics (GIW 2005). In 2008, he received the Best Poster Award in the 12th Annual International Conference Research in Computational Molecular Biology (RECOMB 2008). In 2011, he received the Best Paper Runner-Up Award of the 16th International Conference on Database Systems for Advanced Applications (DASFAA 2011). He also won two Best Performance Awards in international benchmarking competitions, i.e. Dialogue for Reverse Engineering Assessments and Methods (DREAM) 2007 USA and EU Activity Recognition Challenge 2011.

Efficiently detecting switching mechanisms in gene expression

Hiroshi Mamitsuka
Kyoto University

Biological phenomena are complex and hard to understand entirely. However, there exist simple but interesting systems made by a relatively small number of biological components. In this talk I will raise one typical example, which we call “switching mechanism” in gene expression, where two genes are either positively or negatively correlated with each other, depending on given two conditions. I will first explain biological background behind this mechanism and introduce known methods for finding this mechanism from gene expression datasets and possible problems in these approaches. I will then propose techniques to overcome those existing problems and show experimental results obtained by applying the proposed approaches to the problem of finding the switching mechanism from expression data, under synthetic and real data settings.

Brief bio. Hiroshi Mamitsuka received the B.S. degree in biophysics and biochemistry, the M.E. degree in information engineering, and the Ph.D degree in information sciences from the University of Tokyo, in 1988, 1991 and 1999, respectively. He is now a full professor of Kyoto University. His current research interests include mining from graphs and networks in biology and chemistry.

Cancer Gene Network Analysis

Satoru Miyano
University of Tokyo

Cancer is a very complex disease that occurs from accumulation of multiple genetic and epigenetic changes in individuals who carry different genetic backgrounds and have suffered from distinct carcinogen exposures. These changes affect various pathways which are necessary for normal biological activities and gene networks are driving these pathways in disorder in the center. By intensively using the supercomputer system of the Human Genome Center (225TFLOPS at peak) and K computer (10PFLOPS at benckmark) at RIKEN Advanced Institute of Computational Science, we are challenging for development of systematic methodology for unraveling gene networks and their diversity lying over genetic variations, mutations, environments and diseases. We first present a statistical/computational method that will exhibit how gene networks vary from patient to patient based on gene expression profiles according to a modulator, which is any score representing characteristics of cells, e.g. survival. We defined an EMT (epithelial-mesenchymal transition) modulator and analyzed gene expression profiles of 762 cancer cell lines. Network analysis unraveled global changes of networks with 13,508 genes of different EMT levels. By focusing on E-cadherin, 24 genes were predicted as its regulator, of which 12 have been reported in the literature. A novel EMT regulator KLF5 was also discovered in this study. We also analyzed Erlotinib resistant networks using 160 NSCLCs with GI50 as a modulator. Hubness analysis exhibited that NKX2-1/TTF-1 is the key gene for Erlotinib resistance in NSCLCs. Our microRNA/mRNA gene network analysis with Bayesian network method also revealed subnetworks with hub genes (including NKX2-1/TTF-1) that may switch cancer survival. We also developed a statistical/computational method for modeling dynamics in cancer cells from time-course gene expression profiles and revealed dynamic network changes against anti-cancer drugs and network differences between drug-sensitive and drug-

resistant cancer cells. We devised a state space model (SSM) with dimension reduction method for reverse-engineering gene networks from time-course data, with which we can view their dynamic changes over time by simulation. We succeeded in computing a gene network with prediction ability focused on 1500 genes from data of about 20 time-points after EGF stimulation with/without Gefitinib dose. We applied this SSM model to human normal lung cell treated with (case)/without (control) Gefitinib, and we identified genes under differential regulations between case and control. This signature of genes was used to predict prognosis for lung cancer patients and showed a good performance for survival prediction. On-going cancer research using K computer is also introduced.

Brief bio. Satoru Miyano is a professor at the Human Genome Center, Institute of Medical Science, The University of Tokyo. He received the B.S., M.S. and Ph.D. all in Mathematics from Kyushu University, Japan, in 1977, 1979 and 1984, respectively. He joined Human Genome Center in 1996. The recent advances in biomedical research have been producing large-scale, ultra-high dimensional, ultra-heterogeneous data. His mission is to create computational strategy for systems biology and medicine towards translational bioinformatics. He is well known for his research on gene network analysis, modeling and simulation of biological systems, and peta flops computing for biomedical applications.

Accepted Papers

The accepted papers can be downloaded from http://tinyurl.com/giw2013/accepted-papers.

1. Hufeng Zhou, Javad Rezaei, Willy Hugo, Shangzhi Gao, Jingjing Jin, Mengyuan Fan, Chern-Han Yong, Michal Wozniak and Limsoon Wong. "Stringent DDI-based Prediction of H. sapiens-M. tuberculosis H37Rv Protein-Protein Interactions". BMC Systems Biology, 7(Suppl 6):S6, 2013
5. Jing-Doo Wang. "Comparing virus classification using genomic materials according to different taxonomic levels". JBCB, 11(6):1343003, 2013
8. Liang Zhao, Steven C. H. Hoi, Zhenhua Li, Limsoon Wong, Hung Nguyen, Jinyan Li. "Coupling graphs, efficient algorithms and B-cell epitope prediction". TCBB, to appear
9. Slavka Jaromerska, Petr Praus and Young-Rae Cho. "Distance-wise pathway discovery from protein-protein interaction networks weighted by semantic similarity". JBCB, 12(1):1450004, 2014
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68. Laleh Soltan Ghoraie, Forbes Burkowski, Shuai

Cheng Li and Mu Zhu. "Residue-specific side-chain polymorphisms via particle belief propagation". TCBB, to appear

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84. Sriganesh Srihari, Venkatesh Raman, Hon Wai Leong and Mark A. Ragan. "Evolution and controllability of cancer networks: A Boolean perspective". TCBB, to appear

89. Venkata Rajesh Yella and Manju Bansal. "DNA structural features and architecture of promoter regions play a role in gene responsiveness of S. cerevisiae". JBCB, 11(6):1343001, 2013

91. Igor I. Titov and Pavel S. Vorozheykin. "Ab initio human miRNA and pre-miRNA prediction". JBCB, 11(6):1343009, 2013

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98. Henry Han, Xiao-Li Li, See-Kiong Ng and Zhou Ji. "Multi-resolution test for consistent phenotype discrimination and biomarker discovery in translational bioinformatics". JBCB, 11(6):1343010, 2013

Accepted Posters

The accepted posters can be downloaded from http://tinyurl.com/giw2013/accepted-posters.

1. Kirubakaran Palani and Karthikeyan Muthusamy. "Molecular dynamics simulation of the interaction between TNKS1/TNKS2 and IWR1 inhibitor"
2. Trees-Juen Chuang, Feng-Chi Chen and Yen-Zho Chen. "DNA methylation is differentially correlated with exonic evolutionary rates in a position-dependent manner"
3. Jiangyu Li, Yiqing Mao, Xiaolei Wang, Yang Liu and Dongsheng Zhao. "A fast microorganism detection algorithm based on high-throughput sequencing data"
4. Hiroki Miyashita, Yoshio Kuroki and Norio Matsushima. "Novel leucine rich repeats"
5. Ryoichi Minai, Tsuyoshi Waku and Shoji Makino. "Gene network estimation by using information of transcription factor binding DNA sequence and microarray data from many samples"
6. Ai Muto, Katsuhisa Ozaki, Susumu Goto and Masaaki Kotera. "Development of lepidopteran insect ortholog database"
7. Kazuhiro Maeda and Hiroyuki Kurata. "Multiparameter sensitivity as a robustness measure for dynamic biochemical models"
8. Ben-Yang Liao and Meng-Pin Weng. "Genomic evidence for the importance of gene expression at transcription level in determining mammalian phenotypes"
9. Shuichi Yoshida, Sunao Kaneko and Takuhiro Nishio. "A computational approach for predicting SCN1A-related epilepsy phenotypes based on physico-chemical property changes"
10. Kazuhiro Takemotow and Kaori Kihara. "Association between modular organization of cancer signaling networks and patient survivability"
11. Ikuko Nishikawa, Tomoki Ishino, Yukako Tohsato, Shuichi Onami, Satoshi Fukuchi and Ken Nishikawa. "Predicting human protein phosphorylation sites in intrinsically disordered region by support vector machine"
12. Naoki Nariai, Osamu Hirose, Kaname Kojima, Kazuko Ueno and Masao Nagasaki. "Comparative assessment of computational methods for

quantifying mammalian transcript isoforms from RNA-Seq data"

13. Kentaro Inoue, Hisaaki Shinohara and Mariko Okada-Hatakeyama. "Dynamic modeling of NF-kappaB signaling system in B cell"
14. Lina Ma, Ang Li, Dong Zou and Zhang Zhang. "Harnessing community intelligence in collaborative curation of human long non-coding RNAs"
15. Takuma Shirahase, Takayoshi Tomono, Hisao Kojima, Yukako Tohsato and Masahiro Ito. "Sequence analysis of intrinsically disordered region of nucleus related human O-GlcNAcylated protein"
16. Takayoshi Tomono, Hisao Kojima, Yukako Tohsato and Masahiro Ito. "A study of glycan evolution by comprehensive analysis of human glycosyltransferases using phylogenetic profiling"
17. Jiwoong Seok, Seongbeom Cho and Myungguen Chung. "Stand-alone LiveCD system for high-throughput gene expression regulation associate analysis"
18. Ipputa Tada, Seikoh Saitoh, Hiroaki Aoyama, Eisuke Kuraya, Shoya Arakawa, Hiroyuki Iha, Naoya Shinzato and Shinya Ikematsu. "Genomics of a lactic acid bacteria isolated from the Okinawan natural environment"
19. Aditya Kumar and Manju Bansal. "Role of DNA sequence dependent structural properties in gene expression"
20. Masao Nagasaki, Naoki Nariai, Kaname Kojima, Yumi Yamaguchi, Yukuto Sato, Riu Yamashita, Junya Yamagishi, Ikuko Motoike, Matsuyuki Shirota, Kengo Kinoshita, Jun Yasuda, Fukumi Katsuoka and Masayuki Yamamoto. "Thousands Japanese whole genome sequencing and bioinformatics at Tohoku Medical Megabank Organization"
21. Yushi Takahashi and Kiyoko F. Aoki-Kinoshita. "GlycomeAtlas: A visualization tool of glycan structure expression in human and mouse"
22. Koji Masuda, Claire Renard-Guillet, Takashi Sutani, Ryuichiro Nakato, Yuki Katou, Atsunori Yoshimura, Yutaka Kanoh, Hisao Masai and Katsuhiko Shirahige. "Replication initiation is associated to divergent promoter regions in Schizosaccharomyces pombe genome"
23. Kaname Kojima, Naoki Nariai, Takahiro Mimori, Mamoru Takahashi, Yumi Yamaguchi-Kabata, Yukuto Sato and Masao Nagasaki. "Performance evaluation of variant calling methods with or without pedigree information"
24. Jiwoong Seok, Kijin Yu and Seongbeom Cho. "PAGED: Application for protein-protein-interaction analysis with gene expression data"
25. R. Rakshambikai, N. Srinivasan and Rupali A. Gadkari. "Analysis of extended kinome of zebrafish with immensely over represented PIM kinase subfamily"
26. Akitaka Shionoya, Kunihiko Ikuta, Shuichi Onami, Masahiro Ito and Yukako Tohsato. "Large-scale kinetic modeling for the central metabolism in Escherichia coli grown on glucose or glycerol"
27. B. Lakshmi, G. Archunan and N. Srinivasan. "Conservation of conformational changes upon ligand binding in homologous lipocalins"
28. Naruemon Pratanwanich and Pietro Lio'. "Bayesian matrix factorisation for learning latent pathway inter-dependencies and identifying responsive pathways"
29. Yuki Kato, Jakob Hull Havgaard and Jan Gorodkin. "Fast RNA structural comparison using coarse-grained base-pairing probabilities"
30. Zhang Zhang. "Community curation in the era of big data"
31. Akihiro Fujita and Kiyoko F. Aoki-Kinoshita. "Development of an algorithm to analyze atomic structures of glycan"
32. Yi-Hui Lin and Jiun-Ysn Huang. "Dysconnection of functional network in Schizophrenia: A ROI-based model approach"
33. Chandana Tennakoon, Jing-Quan Lim and Wing-Kin Sung. "Fast and accurate alignment with BatAlign"
34. Manabu Sugii, Adrien Faure and Hiroshi Matsuno. "A design method of artificial genetic circuits on effective search of these logical structures"
35. Rajesh Yella and Manju Bansal. "The relationship between transcription pre-initiation complexes and gene expression variability in S. cerevisiae"
36. Yukako Tohsato, Kenneth Ho, Koji Kyoda and Shuichi Onami. "SSBD: An integrated database for Systems Science of Biological Dynamics"
37. Naoaki Ono, Yuki Okuda, Masanori Arita, Daisaku Ohota, Tetsuo Sato, Tadao Sugiura, Md. Altaf-UI Amin and Shigehiko Kanaya. "Evaluation of transcriptome assembly platforms for RNA-seq method using non-model organisms"

38. Sophie Octavia, Qinning Wang, Sandeep Kaur, Vitali Sintchenko, Gwendolyn L Gilbert and Ruiting Lan. "Applicability of high-throughput genome sequencing to analyse a Salmonella enterica serovar Typhimurium DT170 outbreak"
39. Huy Hoang Do and Wing Kin Sung. "Small and fast data format for genomic numerical signals"
40. Mikhail Matz. "Gene Ontology analysis of continuous measures based on Mann-Whitney U test with adaptive clustering of GO categories"
41. Kazunori Waki and Hideo Matsuda. "Causal discovery from omics information using Bayesian network"
42. Nataly S. Safronova, Ekaterina V. Kulakova and Yuriy L. Orlov. "Applications of text complexity measures to genome sequences analysis"
43. Sriganesh Srihari, Chao Liu, Atefeh Taherian-Fard, Peter T. Simpson, Mark A. Ragan and Kum Kum Khanna. "Harnessing DNA damage repair pathways in breast cancer therapy: A synthetic lethality paradigm"
44. Saloni Agrawal, Asif Javed and Pauline C. Ng. "Combining phenotypic and genotypic data in implicating genes associated with rare disorders"

Conference Venue

GIW2013 is held during 16 to 18 December in the Exploration Theatrette and the Creation Theatrette on Level 4, Matrix, Biopolis. The address of Matrix is: 30 Biopolis Street, Singapore 138671.

Getting to the Matrix, Biopolis. Biopolis is a comfortable 10-minute walk, directly across from the Buona Vista MRT Station. The Buona Vista MRT Station serves the Circle Line and the East-West Line.

Welcome Reception Venue

The GIW2013 Welcome Reception is at 6.15pm on 16 December 2013. The venue is Penang Place, located in the basement of the Connexis building in Fusionopolis. The address is: 1 Fusionopolis Way, Connexis #B1-20. Tel: 6467 7003. The restaurant is famed for its nonya cuisine, which is the cuisine of the Peranakan Chinese that settled into our part of the world in the 15th century.

Getting to Penang Place. Fusionopolis is a short 15 minutes walk from Biopolis. Walk from Matrix to North Buona Vista Rd, turn left and walk along North Buona Vista Rd. When you see Insead, turn right into Ayer Rajah Ave. Connexis is next to Insead.

We will walk as a group from Biopolis to Fusionopolis. The first departure will at 5.45pm. The second departure will be at 5.55pm.

Conference Banquet Venue

The GIW2013 Conference Banquet is at 7pm on 17 December 2013. The venue is The Jewel Box, located on Mount Faber. The address is: 109 Mount Faber Road. Tel: +65 6270 8855. The restaurant is famed for its exquisite panoramic view of Singapore and great embience.

Getting to Jewel Box. If you are going on your own, a nice way to get to The Jewel Box is taking the MRT to the HarbourFront MRT Station, then board a cable car at HarbourFront Tower 2, 15th Floor, Jewel Cable Car Station, after purchasing the cable car ticket on of the ground floor of Tower 2.

We will go as a group from Biopolis to Mount Faber on pre-arranged buses. The buses will depart from Biopolis at 6.00pm.

Recommended Hotel

The hotel nearest to Biopolis is Hotel Park Avenue Rochester. It is next to the Buona Vista MRT Station, 10 minutes walk across the street from Biopolis. The address is: 31 Rochester Drive. Tel: 6808 8600.


Hotel Park Ave @ Rochester
Matrix @ Biopolis
Connexis @ Fusionopois
Buona Vista (EW21)
Buona Vista (CC22)
The Star
The Metropolis (U/C)
MOE Bldg
Rochester Pk
Exchange Green
Rochester Dr
North Buona Vista Rd
Buona Vista Dr
Biopolis Way
Helios
Nanos
Chromos
Centros
Matrix
BIOPOLIS
Proteos
Genome
Neuros
Immun
Nucleos (U/C)
Synapse
Amnios
Biomedical Gr
Biopolis Dr
Biopolis Rd
Biopolis St
NTU@ one-north
NTU Alumni Clubhouse
One-North Pk
One-North Lk
One-North Gateway
Slim Barracks Rise
Anglo-Chinese Jnr College
Fairfield Methodist Sch (Pri)
Aldersgate Meth Ch
Portsdown Rd
Portsdown Cres
Nepal Pk
Pixel
FUSIONOPOLIS
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Connexis
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Weyhill Cl
Dover Rd
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Synthesis (U/C)
Nexus @One-North (U/C)
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