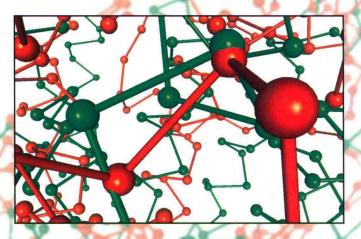
Proceedings of the 5th Asia-Pacific

BIOINFORMATICS

Conference

editors

David Sankoff Lusheng Wang Francis Chin



Proceedings of the 5th Asia-Pacific

BIOINFORMATICS

Conference

Hong Kong

15 - 17 January 2007

Editors

David Sankoff

University of Ottawa, Canada

Lusheng Wang

City University of Hong Kong, Hong Kong

Francis Chin

The University of Hong Kong, Hong Kong

Published by

Imperial College Press 57 Shelton Street Covent Garden London WC2H 9HE

Distributed by

World Scientific Publishing Co. Pte. Ltd. 5 Toh Tuck Link, Singapore 596224

USA office: 27 Warren Street, Suite 401-402, Hackensack, NJ 07601 UK office: 57 Shelton Street, Covent Garden, London WC2H 9HE

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

PROCEEDINGS OF THE 5TH ASIA-PACIFIC BIOINFORMATICS CONFERENCE

Copyright © 2007 by Imperial College Press

All rights reserved. This book, or parts thereof, may not be reproduced in any form or by any means, electronic or mechanical, including photocopying, recording or any information storage and retrieval system now known or to be invented, without written permission from the Publisher.

For photocopying of material in this volume, please pay a copying fee through the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923, USA. In this case permission to photocopy is not required from the publisher.

ISBN-13 978-1-86094-783-4 ISBN-10 1-86094-783-2

Printed in Singapore by B & JO Enterprise

Proceedings of the 5th Asia-Pacific

BIOINFORMATICS

Conference

SERIES ON ADVANCES IN BIOINFORMATICS AND COMPUTATIONAL BIOLOGY

Series Editors:

ISSN: 1751-6404

Ying XU (University of Georgia, USA) Limsoon WONG (National University of Singapore, Singapore)

Associate Editors:

Ruth Nussinov (NCI, USA) Rolf Apweiler (EBI, UK) Ed Wingender (BioBase, Germany) See-Kiong Ng (Inst for Infocomm Res, Singapore) Kenta Nakai (Univ of Tokyo, Japan) Mark Ragan (Univ of Queensland, Australia)

- Vol. 1: Proceedings of the 3rd Asia-Pacific Bioinformatics Conference Eds: Yi-Ping Phoebe Chen and Limsoon Wong
- Vol. 2: Information Processing and Living Systems Eds: Vladimir B. Bajic and Tan Tin Wee
- Vol. 3: Proceedings of the 4th Asia-Pacific Bioinformatics Conference Eds: Tao Jiang, Ueng-Cheng Yang, Yi-Ping Phoebe Chen and Limsoon Wong
- Vol. 4: Computational Systems Bioinformatics Eds: Peter Markstein and Ying Xu
- Vol. 5: Proceedings of the 5th Asia-Pacific Bioinformatics Conference Eds: David Sankoff, Lusheng Wang and Francis Chin

PREFACE

High-throughput sequencing and functional genomics technologies have given us the human genome sequence as well as those of other experimentally, medically and agriculturally important species, and have enabled large-scale genotyping and gene expression profiling of human populations. Databases containing large numbers of sequences, polymorphisms, structures and gene expression profiles of normal and diseased tissues are rapidly being generated for human and model organisms. Bioinformatics is thus rapidly growing in importance in the annotation of genomic sequences, in the understanding of the interplay among and between genes and proteins, in the analysis the genetic variability of species, in the identification of pharmacological targets and in the inference of evolutionary origins, mechanisms and relationships.

The Asia-Pacific Bioinformatics Conference series is an annual forum for exploring research, development, and novel applications of bioinformatics. It brings together researchers, professionals, and industrial practitioners for interaction and exchange of knowledge and ideas. The Fifth Asia-Pacific Bioinformatics Conference, APBC2007, was held in Hong Kong 15–17 January, 2007.

A total of 104 papers were submitted to APBC 2007. These submissions came from Bangladesh, China, Hong Kong, India, Japan, Korea, Malaysia, Singapore, Taiwan, Thailand, Australia, New Zealand, Denmark, France, Germany, Hungary, Italy, Israel, Portugal, UK, Canada, Mexico and USA. We assigned each paper to at least three members of the programme committee. Although not all members of the programme committee managed to review all the papers assigned to them, a total of 317 reviews were received, so that there were about three reviews per paper on average.

A total of 35 papers (33%) were accepted for presentation and publication in the proceedings of APBC 2007. Based on the affiliation of the authors, 1.25 of the accepted papers were from China, 1.46 were from Hong Kong, 3 were from Japan, 0.83 were from Korea, 1 were from Singapore, 2.30 were from Australia, 2 were from Denmark, 0.15 were from France, 4.5 were from Germany, 0.5 were from Italy, 1 were from Portugal, 1.66 were from UK, 4.57 were from Canada, 10.78 were from USA.

In addition to the accepted papers, the scientific programme of APBC 2006 also included three keynote talks, by Jennifer A. Marshall Graves, Joseph H. Nadeau and Pavel A. Pevzner, as well as tutorial and poster sessions. The presentations were of very high quality. Almost a third focused on evolution and phylogeny, largely at the genome level, a similar number dealt with protein structure and proteomics more generally, and a good proportion studied various aspects of pathways,

networks, transcriptomics and microarray technology. A range of other topics in bioinformatics and computational biology were also covered, ranging from motif and gene recognition, through haplotypes and population genetics, to databases and text mining. Much of this work featured techniques of sequence analysis, while many of the papers included applications to biology and medicine.

We had a great time in Hong Kong, enhancing the interactions between many researchers and practitioners, and reuniting the Asia-Pacific bioinformatics community in the context of an international conference with worldwide participation.

Finally, we wish to express our gratitude to the authors of the submitted papers, the members of the programme committee and their subreferees, the members of the organizing committee, Phoebe Chen and Limsoon Wong (our liaisons in the APBC steering committee), the keynote speakers, our generous sponsors, and supporting organizations for making APBC 2007 a great success.

David Sankoff Lusheng Wang Francis Chin

17 January 2007

${ m APBC2007} \ { m ORGANIZATION}$

Conference Chair

Francis YL Chin, The University of Hong Kong, Hong Kong

Organizing Committee

Francis YL Chin (Chair), The University of Hong Kong
David Smith (Poster Session), The University of Hong Kong
H.F. Ting (Finance and Registration), The University of Hong Kong
Lusheng Wang (Publication), The City University of Hong Kong
Xiaowen Liu (Publication), The City University of Hong Kong
S.M. Yiu (Local Arrangement and Tutorial), The University of Hong Kong
Daniel Hung (Webmaster), The University of Hong Kong
Samson Sin (Webmaster), The University of Hong Kong

Steering Committee

Phoebe Chen (Chair), Deakin University, Australia Sang Yup Lee, KAIST, Korea Satoru Miyano, University of Tokyo, Japan Mark Ragan, University of Queensland, Australia Limsoon Wong, National University of Singapore

Program Committee

David Sankoff (Chair), The University of Ottawa Lusheng Wang (Chair), The City University of Hong Kong Tatsuya Akutsu, Kyoto University Miguel Andrade, Ottawa Health Research Institute Stephane Aris-Brosou, University of Ottawa Joel Bader, Johns Hopkins University Serafim Batzoglou, Stanford University David Bryant, University of Auckland Jeremy Buhler, Washington University in St. Louis Peter Donnelly, University of Oxford Dannie Durand, Carnegie Mellon University Nadia El-Mabrouk, University of Montreal Robert Giegerich, Bielefeld University Carole Goble, University of Manchester Concettina Guerra, Universita' di Padova Dan Gusfield, University of California, Davis Michael Hallett, McGill University Sridhar Hannenhalli, University of Pennsylvania Daniel Huson, Tbingen University Gavin Huttley, Australian National University Jenn-Kang Hwang, National Chiao Tung University Tao Jiang, University of California - Riverside Uri Keich, Cornell University Anand Kumar, University of Leipzig Tak Wah Lam, The University of Hong Kong Doheon Lee, KAIST, Korea Jinyan Li, Institute for Infocomm Research Wentian Li, Feinstein Institute for Medical Research Guohui Lin, University of Alberta Michal Linial, The Hebrew University of Jerusalem Zhijie Liu, University of Georgia Bin Ma, University of Western Ontario Satoru Miyano, The University of Tokyo Laxmi Parida, IBM Thomas J. Watson Research Center Mark Ragan, University of Queensland Marie-France Sagot, University Claude Bernard, Lyon I Akinori Sarai, Kyushu Institute of Technology Vincent Schachter, Genoscope Steven Skiena, State University of New York at Stony Brook Edward Susko, Dalhousie University Yun Song, University of California, Davis Robert Stevens, University of Manchester Alfonso Valencia, Centro Nacional de Biotechnologia Michael Waterman, University of Southern California

Ken Wolfe, University of Dublin Stacia Wyman, Williams College Hong Yan, City University of Hong Kong Qiang Yang, Hong Kong University of Science and Technology Kaizhong Zhang, University of Western Ontario Liqing Zhang, Virginia Tech Louxin Zhang, National University of Singapore

Additional Reviewers

Shandar Ahmad Iris Bahir Shihven Chen Tobias Dezulian James Eales Morihiro Havashida Helen Hulme Gunnar W. Klau Jingping Liu Julia Mixtacki Hiroshi Nakashima Magnus Rattray Baozhen Shan Ashish V. Tendulkar Balaji Venkatachalam Katy Wolstencroft Zheng Yuan

Marcos Jesus Arauzo Bravo Richard Bean Matteo Comin Zhihong Ding Logan Everett Cornelia Hedeler Shane Jensen Kiyoung Lee Yaniv Loewenstein Jose Carlos Nacher Kav Nieselt Jonathan Schug Yun S. Song Victor Tong Li-San Wang Yufeng Wu Guanglan Zhang

Alexander Auch Pierre-Yves Bourguignon Mike Cornell Maxime Durot Paul Fisher Duncan Hull Noam Kaplan Yaoyong Li Suryani Lukman Niranjan Nagarajan Elon Portugaly Charles Semple Kristian Stevens Roy Varshavsky Michael Wilson Lei Xin

CONTENTS

Preface	v
APBC 2007 Organization	vii
Keynote Papers	
Exploring Genomes of Distantly Related Mammals J.A. Marshall Graves	1
Bugs, Guts and Fat - A Systems Approach to the Metabolic 'Axis of Evil' $J.\ Nadeau$	3
Protein Identification via Spectral Networks Analysis P. Pevzner	5
Contributed Papers	
Metagenome Analysis using MEGAN D.H. Huson, A.F. Auch, J. Qi, and S.C. Schuster	7
Algorithmic Approaches to Selecting Control Clones in DNA Array Hybridization Experiments Q. Fu, E. Bent, J. Borneman, M. Chrobak, and N. Young	17
Subtle Motif Discovery for Detection of DNA Regulatory Sites M. Comin, and L. Parida	27
An Effective Promoter Detection Method using the Adaboost Algorithm X. Xie, S. Wu, KM. Lam, and H. Yan	37
A New Strategy of Geometrical Biclustering for Microarray Data Analysis H. Zhao, A.W.C. Liew, and H. Yan	47

Using Formal Concept Analysis for Microarray Data Comparison V. Choi, Y. Huang, V. Lam, D. Potter, R. Laubenbacher, and K. Duca	57
An Efficient Biclustering Algorithm for Finding Genes with Similar Patterns in Time-series Expression Data S.C. Madeira, and A.L. Oliveira	67
Selecting Genes with Dissimilar Discrimination Strength for Sample Class Prediction Z. Cai, R. Goebel, M.R. Salavatipour, Y. Shi, L. Xu, and G. Lin	81
Computing the All-Pairs Quartet Distance on a Set of Evolutionary Trees M. Stissing, T. Mailund, C.N.S. Pedersen, G.S. Brodal, and R. Fagerberg	91
Computing the Quartet Distance Between Evolutionary Trees of Bounded Degree M. Stissing, C.N.S. Pedersen, T. Mailund, G.S. Brodal, and R. Fagerberg	101
A Global Maximum Likelihood Super-Quartet Phylogeny Method P. Wang, B.B. Zhou, M. Taraeneh, D. Chu, C. Wang, A.Y. Zomaya, and R.P. Brent	111
A Randomized Algorithm for Comparing Sets of Phylogenetic Trees SJ. Sul, and T.L. Williams	121
Protein Structure-Structure Alignment with Discrete Fréchet Distance M. Jiang, Y. Xu, and B. Zhu	131
Deriving Protein Structure Topology from the Helix Skeleton in Low Resolution Density Map using Rosetta Y. Lu, J. He, and C.E.M. Strauss	143
Fitting Protein Chains to Cubic Lattice is NP-Complete J. Maňuch, and D.R. Gaur	153
Inferring a Chemical Structure from a Feature Vector Based on Frequency of Labeled Paths and Small Fragments T. Akutsu, and D. Fukagawa	165

277

Pathway Detection

F. Hüffner, S. Wernicke, and T. Zichner

De Novo Peptide Sequencing for Mass Spectra Based on Multi-Charge Strong Tags	287
K. Ning, K.F. Chong, and H.W. Leong	
Complexities and Algorithms for Glycan Structure Sequencing using Tandem Mass Spectrometry B. Shan, B. Ma, K. Zhang, and G. Lajoie	297
Semi-supervised Pattern Learning for Extracting Relations from Bioscience Texts S. Ding, M. Huang, and X. Zhu	307
Flow Model of the Protein-protein Interaction Network for Finding Credible Interactions K. Okada, K. Asai, and M. Arita	317
All Hits All The Time: Parameter Free Calculation of Seed Sensitivity D.Y.F. Mak, and G. Benson	327
Fast Structural Similarity Search Based on Topology String Matching SH. Park, D. Gilbert, and K.H. Ryu	341
Simple and Fast Alignment of Metabolic Pathways by Exploiting Local Diversity S. Wernicke, and F. Rasche	353
Combining N-grams and Alignment in G-protein Coupling Specificity Prediction B. Y.M. Chen, and J.G. Carbonell	363
Author Index	373

EXPLORING GENOMES OF DISTANTLY RELATED MAMMALS

JENNIFER A. MARSHALL GRAVES

ARC Centre for Kangaroo Genomics, Research School of Biological Sciences Australian National University, Canberra, ACT 2601, Australia

There are three groups of extant mammals, two of which abound in Australia. Marsupials (kangaroos and their relatives) and monotremes (echidna and the fabulous platypus) have been evolving independently for most of mammalian history. The genomes of marsupial and monotreme mammals are particularly valuable because these alternative mammals fill a phylogenetic gap in vertebrate species lined up for exhaustive genomic study. Human and mice (~70MY) are too close to distinguish signal, whereas mammal/bird comparisons (~310MY) are too distant to allow alignment. Kangaroos (180 MY) and platypus (210 MY) are just right. Sequence has diverged sufficiently for stringent detection of homologies that can reveal coding regions and regulatory signals. Importantly, marsupials and monotremes share with humans many mammal-specific developmental pathways and regulatory systems such as sex determination, lactation and X chromosome inactivation.

The ARC Centre for Kangaroo Genomics is characterizing the genome of the model Australian kangaroo Macropus eugenii (the tammar wallaby), which is being sequenced by AGRF in Australia, and Baylor (funded by NIH) in the US. We are developing detailed physical and linkage maps of the genome to complement sequencing, and will prepare and array cDNAs for functional studies, especially of reproduction and development. Complete sequencing of the distantly related Brazilian short-tailed opossum Monodelphis domestica by the NIH allows us to compare distantly related marsupials. Sequencing of the genome of the platypus, Ornithorhynchus anatinus by Washington University (funded by the NIH) is complete, and our lab is anchoring contigs to the physical map. We have isolated and completely characterized many BACs and cDNAs containing kangaroo and platypus genes of interest, and demonstrate the value of comparisons to reveal conserved genome organization and function, and new insights in the evolution of the mammalian genome, particularly sex chromosomes.