**About this Series**

The series “Advances in Intelligent Systems and Computing” contains publications on theory, applications, and design methods of Intelligent Systems and Intelligent Computing. Virtually all disciplines such as engineering, natural sciences, computer and information science, ICT, economics, business, e-commerce, environment, healthcare, life science are covered. The list of topics spans all the areas of modern intelligent systems and computing.

The publications within “Advances in Intelligent Systems and Computing” are primarily textbooks and proceedings of important conferences, symposia and congresses. They cover significant recent developments in the field, both of a foundational and applicable character. An important characteristic feature of the series is the short publication time and world-wide distribution. This permits a rapid and broad dissemination of research results.

**Advisory Board**

**Chairman**

Nikhil R. Pal, Indian Statistical Institute, Kolkata, India  
e-mail: nikhil@isical.ac.in

**Members**

Rafael Bello, Universidad Central “Marta Abreu” de Las Villas, Santa Clara, Cuba  
e-mail: rbellop@uclv.edu.cu

Emilio S. Corchado, University of Salamanca, Salamanca, Spain  
e-mail: escorchado@usal.es

Hani Hagras, University of Essex, Colchester, UK  
e-mail: hani@essex.ac.uk

László T. Kóczy, Széchenyi István University, Győr, Hungary  
e-mail: koczy@sze.hu

Vladik Kreinovich, University of Texas at El Paso, El Paso, USA  
e-mail: vladik@utep.edu

Chin-Teng Lin, National Chiao Tung University, Hsinchu, Taiwan  
e-mail: ctlin@mail.nctu.edu.tw

Jie Lu, University of Technology, Sydney, Australia  
e-mail: Jie.Lu@uts.edu.au

Patricia Melin, Tijuana Institute of Technology, Tijuana, Mexico  
e-mail: epmelin@hafsamx.org

Nadia Nedjah, State University of Rio de Janeiro, Rio de Janeiro, Brazil  
e-mail: nadia@eng.uerj.br

Ngoc Thanh Nguyen, Wroclaw University of Technology, Wroclaw, Poland  
e-mail: Ngoc-Thanh.Nguyen@pwr.edu.pl

Jun Wang, The Chinese University of Hong Kong, Shatin, Hong Kong  
e-mail: jwang@mac.cuhk.edu.hk
Preface

Biological and biomedical research are increasingly driven by experimental techniques that challenge our ability to analyse, process and extract meaningful knowledge from the underlying data. The impressive capabilities of next generation sequencing technologies, together with novel and ever evolving distinct types of omics data technologies, have put an increasingly complex set of challenges for the growing fields of Bioinformatics and Computational Biology. To address the multiple related tasks, for instance in biological modeling, there is the need to, more than ever, create multidisciplinary networks of collaborators, spanning computer scientists, mathematicians, biologists, doctors and many others.

The International Conference on Practical Applications of Computational Biology & Bioinformatics (PACBB) is an annual international meeting dedicated to emerging and challenging applied research in Bioinformatics and Computational Biology. Building on the success of previous events, the 8th edition of PACBB Conference will be held on 4–6 June 2014 in the University of Salamanca, Spain. In this occasion, special issues will be published by the Journal of Integrative Bioinformatics, the Journal of Computer Methods and Programs in Biomedicine and the Current Bioinformatics journal covering extended versions of selected articles.

This volume gathers the accepted contributions for the 8th edition of the PACBB Conference after being reviewed by different reviewers, from an international committee composed of 72 members from 15 countries. PACBB’14 technical program includes 34 papers from about 16 countries of origin, spanning many different sub-fields in Bioinformatics and Computational Biology.

Therefore, this event will strongly promote the interaction of researchers from diverse fields and distinct international research groups. The scientific content will be challenging and will promote the improvement of the valuable work that is being carried out by the participants. Also, it will promote the education of young scientists, in a post-graduate level, in an interdisciplinary field.

We would like to thank all the contributing authors and sponsors (Telefónica Digital, Indra, Ingeniería de Software Avanzado S.A, IBM, JCyL, IEEE Systems Man and Cybernetics Society Spain, AEPIA Asociación Española para la Inteligencia Artificial, APPIA Associação Portuguesa Para a Inteligência Artificial, CNRS Centre national
de la recherche scientifique), AI*IA, as well as the members of the Program Committee and the Organizing Committee for their hard and highly valuable work and support. Their effort has helped to contribute to the success of the PACBB’14 event. PACBB’14 wouldn’t exist without your assistance. This symposium is organized by the Bioinformatics, Intelligent System and Educational Technology Research Group (http://bisite.usal.es/) of the University of Salamanca and the Next Generation Computer System Group (http://sing.ei.uvigo.es/) of the University of Vigo.

Julio Sáez-Rodríguez
Miguel P. Rocha
PACBB’14 Programme Co-chairs

Florentino Fdez-Riverola
Juan F. De Paz Santana
PACBB’14 Organizing Co-chairs
Organization

General Co-chairs

Florentino Fdez-Riverola
University of Vigo, Spain
Juan F. De Paz
University of Salamanca, Spain
Julio Sáez-Rodríguez
European Bioinformatics Institute, United Kingdom
Miguel Rocha
University of Minho, Portugal

Program Committee

Alicia Troncoso
University Pablo de Olavide, Spain
Amparo Alonso
University of A Coruña, Spain
Ana Cristina Braga
University of Minho, Portugal
Anália Lourenço
University of Vigo, Spain
Armando Pinho
University of Aveiro, Portugal
Caludine Chaouiyia
Gulbenkian Institute, Portugal
Camilo Lopez
Universidad Nacional de Colombia, Colombia
Carlos A.C. Bastos
University of Aveiro, Portugal
Daniel Glez-Peña
University of Vigo, Spain
Daniela Correia
CEB, University of Minho, Portugal
David Hoksza
Charles University in Prague, Czech Republic
Eva Lorenzo
University of Vigo, Spain
Fernanda Correia Barbosa
DETI/IEETA, University of Aveiro, Portugal
Fernando Díaz-Gómez
University of Valladolid, Spain
Fidel Cacheda
University of A Coruña, Spain
Florencio Pazos
CNB, Spanish Council for Scientific Research, Spain
Francisco Torres-Avilés
Universidad de Santiago de Chile, Chile
Frank Klawonn-Ostafilia
University of Applied Sciences, Wolfenbuettel, Germany
Gonzalo Gómez-López
UBio/CNIO, Spanish National Cancer Research Centre, Spain
Gustavo Isaza  
Universidad de Caldas, Colombia

Hagit Shatkay  
University of Delaware, USA

Heri Ramampiaro  
Norwegian University of Science and Technology, Norway

Hugo Lópe Fernández  
University of Vigo, Spain

Hugo Miguel Santos  
Universidade Nova de Lisboa, Portugal

Isabel C. Rocha  
IBB/CEB, University of Minho, Portugal

Jiri Novak  
Charles University in Prague, Czech Republic

João Rodrigues  
University of Aveiro, Portugal

Joel P. Arrais  
DEI/CISUC, University of Coimbra, Portugal

Jorge Ramirez  
Universidad Nacional de Colombia, Colombia

Jorge Vieira  
Institute for Molecular and Cell Biology, Portugal

José Antonio Castellanos Garzón  
University of Valladolid, Spain

José Ignacio Requeno  
University of Zaragoza, Spain

José Luis Capelo  
Universidade Nova de Lisboa, Portugal

José Luis Oliveira  
University of Aveiro, Portugal

José Manuel Colom  
University of Zaragoza, Spain

Juan Antonio García Ranea  
University of Malaga, Spain

Julio R. Banga  
IIM, Spanish Council for Scientific Research, Spain

Liliana Lopez-Kleine  
Universidad Nacional de Colombia, Colombia

Loris Nanni  
University of Bologna, Italy

Lourdes Borrajo  
University of Vigo, Spain

Luis F. Castillo  
Universidad de Caldas, Colombia

Luis Figueiredo  
European Bioinformatics Institute, United Kingdom

Luis M. Rocha  
Indiana University, USA

M Alamgir Hossain  
Northumbria University at Newcastle, United Kingdom

Mª Araceli Sanchís de Miguel  
University Carlos III of Madrid, Spain

Manuel Álvarez Díaz  
University of A, Spain

Miguel Reboiro  
University of Vigo, Spain

Mohammad Abdullah Al-Mamun  
Northumbria University, United Kingdom

Mohd Saberi Mohamad  
Universiti Teknologi Malaysia, Malaysia

Monica Borda  
University of Cluj-Napoca, Romania

Narmer Galeano  
Cenicafé, Colombia

Nuno Fonseca  
CRACS/INESC, Porto, Portugal

Nuria Medina Medina  
CITIC, University of Granada, Spain

Pierpaolo Vittorini  
University of L’Aquila, Italy

Reyes Pavón  
University of Vigo, Spain

Rita Ascenso  
Polytecnic Institute of Leiria, Portugal

Rosalía Laza  
University of Vigo, Spain
Rubén López-Cortés  Universidade Nova de Lisboa, Portugal
Rui Brito  University of Coimbra, Portugal
Rui C. Mendes  CCTC, University of Minho, Portugal
Rui Camacho  LIAAD/FEUP, University of Porto, Portugal
Rui Rijo  Polytecnic Institute of Leiria, Portugal
Sara C. Madeira  IST/INESC ID, Lisbon, Portugal
Sara P. Garcia  University of Aveiro, Portugal
Sérgio Deusdado  Polytecnic Institute of Bragança, Portugal
Sergio Matos  DETI/IEETA, University of Aveiro, Portugal
Silas Vilas Boias  University of Auckland, New Zealand
Slim Hammadi  Ecole Centrale de Lille, France
Thierry Lecroq  University of Rouen, France
Tiago Resende  CEB, University of Minho, Portugal
Vera Afreixo  University of Aveiro, Portugal

**Organising Committee**

Juan M. Corchado  University of Salamanca, Spain
Javier Bajo  Polytechnic University of Madrid, Spain
Juan F. de Paz  University of Salamanca, Spain
Sara Rodríguez  University of Salamanca, Spain
Dante I. Tapia  University of Salamanca, Spain
Fernando de la Prieta Pintado  University of Salamanca, Spain
Davinia Carolina Zato Domínguez  University of Salamanca, Spain
Gabriel Villarrubia González  University of Salamanca, Spain
Alejandro Sánchez Yuste  University of Salamanca, Spain
Antonio Juan Sánchez Martín  University of Salamanca, Spain
Cristian I. Pinzón  University of Salamanca, Spain
Rosa Cano  University of Salamanca, Spain
Emilio S. Corchado  University of Salamanca, Spain
Eugenio Aguirre  University of Granada, Spain
Manuel P. Rubio  University of Salamanca, Spain
Belén Pérez Lancho  University of Salamanca, Spain
Angélica González Arrieta  University of Salamanca, Spain
Vivian F. López  University of Salamanca, Spain
Ana de Luís  University of Salamanca, Spain
Ana B. Gil  University of Salamanca, Spain
Mª Dolores Muñoz Vicente  University of Salamanca, Spain
Jesús García Herrero  University Carlos III of Madrid, Spain
Contents

Applications

Agent-Based Model for Phenotypic Prediction Using Genomic and Environmental Data ............................................. 1
Sebastien Alameda, Carole Bernon, Jean-Pierre Mano

NAPROC-13: A Carbon NMR Web Database for the Structural Elucidation of Natural Products and Food Phytochemicals ................. 9
José Luis López-Pérez, Roberto Theron, Esther del Olmo,
Beatriz Santos-Buitrago, José Francisco Adserias, Carlos Estévez,
Carlos García Cuadrado, David Eguiluz López, Gustavo Santos-García

Platform Image Processing Applied to the Study of Retinal Vessels .......... 21
Pablo Chamoso, Luis García-Ortiz, José I. Recio-Rodríguez,
Manuel A. Gómez-Marcos

Data Analysis and Mining

Improving miRNA Classification Using an Exhaustive Set of Features ...... 31
Sherin M. ElGokhy, Tetsuo Shibuya, Amin Shoukry

Designing an Ontology Tool for the Unification of Biofilms Data .............................................................. 41
Ana Margarida Sousa, Maria Olívia Pereira, Nuno F. Azevedo,
Anália Lourenço

BEW: Bioinformatics Workbench for Analysis of Biofilms Experimental Data .......................................................... 49
Gael Pérez Rodríguez, Daniel Glez-Peña, Nuno F. Azevedo,
Maria Olívia Pereira, Florentino Fdez-Riverola, Anália Lourenço
Discrimination of Brazilian Cassava Genotypes (*Manihot esculenta* Crantz) According to Their Physicochemical Traits and Functional Properties through Bioinformatics Tools .............................. 57
Rodolfo Moresco, Virgílio G. Uarrota, Eduardo da C. Nunes, Bianca Coelho, Edna Regina Amante, Vanessa Maria Gervin, Carlos Eduardo M. Campos, Miguel Rocha, Marcelo Maraschin

Proteins

Prediction of Active Residues of $\beta$-galactosidase from *Bacteroides thetaiotaomicron* .................................................. 65
Vladimir Vukić, Dajana Hrnjez, Spasenija Milanović, Mirela Iličić, Katarina Kanurić, Edward Petri

Detection of Intramolecular Tunnels Connecting Sequence of Sites in Protein Structures .................................................. 73
Ondřej Strnad, Barbora Kozlíková, Jiří Sochor

Improving Positive Unlabeled Learning Algorithms for Protein Interaction Prediction .................................................. 81
Doruk Pancaroglu, Mehmet Tan

Finding Class C GPCR Subtype-Discriminating N-grams through Feature Selection .................................................. 89
Caroline König, René Alquézar, Alfredo Vellido, Jesús Giraldo

Sequence Analysis

Geometric Approach to Biosequence Analysis .................................................. 97
Boris Brimkov, Valentin E. Brimkov

Timed and Probabilistic Model Checking over Phylogenetic Trees ........ 105
José Ignacio Requeno, José Manuel Colom

mBWA: A Massively Parallel Sequence Reads Aligner ......................... 113
Yingbo Cui, Xiangke Liao, Xiaoqian Zhu, Bingqiang Wang, Shaoliang Peng

Optimizing Multiple Pairwise Alignment of Genomic Sequences in Multicore Clusters .................................................. 121
Alberto Montañola, Concepció Roig, Porfidio Hernández

High Performance Genomic Sequencing: A Filtered Approach .................................................. 129
German Retamosa, Luís de Pedro, Ivan Gonzalez, Javier Tamames

Vera Afreixo, João M.O.S. Rodrigues, Carlos A.C. Bastos
Mutation Analysis in *PARK2* Gene Uncovers Patterns of Associated Genetic Variants ................................................................. 145
Luísa Castro, José Luís Oliveira, Raquel M. Silva

Heterogeneous Parallelization of Aho-Corasick Algorithm ............ 153
Shima Soroushnia, Masoud Daneshtalab, Juha Plosila, Pasi Liljeberg

**Systems Biology**

High-Confidence Predictions in Systems Biology Dynamic Models ....... 161
Alejandro F. Villaverde, Sophia Bongard, Klaus Mauch, Dirk Müller,
Eva Balsa-Canto, Joachim Schmid, Julio R. Banga

A Parallel Differential Evolution Algorithm for Parameter Estimation in Dynamic Models of Biological Systems ...................................... 173
D.R. Penas, Julio R. Banga, P. González, R. Doallo

A Method to Calibrate Metabolic Network Models with Experimental Datasets ................................................................. 183
Octavio Perez-García, Silas Villas-Boas, Naresh Singhal

Metagenomic Analysis of the Saliva Microbiome with Merlin ............ 191
Pedro Barbosa, Oscar Dias, Joel P. Arrais, Miguel Rocha

Networking the Way towards Antimicrobial Combination Therapies ...... 201
Paula Jorge, Maria Olívia Pereira, Anália Lourenço

A Logic Computational Framework to Query Dynamics on Complex Biological Pathways ............................................................... 207
Gustavo Santos-García, Javier De Las Rivas, Carolyn Talcott

Evaluating Pathway Enumeration Algorithms in Metabolic Engineering Case Studies ................................................................. 215
F. Liu, P. Vilaça, I. Rocha, Miguel Rocha

**Text Mining**

T-HMM: A Novel Biomedical Text Classifier Based on Hidden Markov Models ................................................................. 225
A. Seara Vieira, E.L. Iglesias, L. Borrajo

TIDA: A Spanish EHR Semantic Search Engine .............................. 235
Roberto Costumero, Consuelo Gonzalo, Ernestina Menasalvas

BioClass: A Tool for Biomedical Text Classification ....................... 243
R. Romero, A. Seara Vieira, E.L. Iglesias, L. Borrajo

Chemical Named Entity Recognition: Improving Recall Using a Comprehensive List of Lexical Features .............................. 253
Andre Lamurias, João Ferreira, Francisco M. Couto
Bringing Named Entity Recognition on Drupal Content Management System .................................................. 261
José Ferrnandes, Anália Lourenço

Marky: A Lightweight Web Tracking Tool for Document Annotation .... 269
Martín Pérez-Pérez, Daniel Glez-Peña, Florentino Fdez-Riverola,
Anália Lourenço

A Nanopublishing Architecture for Biomedical Data ..................... 277
Pedro Sernadela, Eelke van der Horst, Mark Thompson, Pedro Lopes,
Marco Roos, José Luís Oliveira

Retrieval and Discovery of Cell Cycle Literature and Proteins by Means
of Machine Learning, Text Mining and Network Analysis ............ 285
Martin Krallinger, Florian Leitner, Alfonso Valencia

Author Index ............................................................. 293