Lecture Notes in Bioinformatics 13346

Subseries of Lecture Notes in Computer Science

Series Editors

Sorin Istrail
Brown University, Providence, RI, USA

Pavel Pevzner
University of California, San Diego, CA, USA

Michael Waterman
University of Southern California, Los Angeles, CA, USA

Editorial Board Members

Søren Brunak
Technical University of Denmark, Kongens Lyngby, Denmark

Mikhail S. Gelfand
IITP, Research and Training Center on Bioinformatics, Moscow, Russia

Thomas Lengauer
Max Planck Institute for Informatics, Saarbrücken, Germany

Satoru Miyano
University of Tokyo, Tokyo, Japan

Eugene Myers
Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Marie-France Sagot
Université Lyon 1, Villeurbanne, France

David Sankoff
University of Ottawa, Ottawa, Canada

Ron Shamir
Tel Aviv University, Ramat Aviv, Tel Aviv, Israel

Terry Speed
Walter and Eliza Hall Institute of Medical Research, Melbourne, VIC, Australia

Martin Vingron
Max Planck Institute for Molecular Genetics, Berlin, Germany

W. Eric Wong
University of Texas at Dallas, Richardson, TX, USA

More information about this subseries at https://link.springer.com/bookseries/5381

Ignacio Rojas · Olga Valenzuela ·
Fernando Rojas · Luis Javier Herrera ·
Francisco Ortuño (Eds.)

Bioinformatics and Biomedical Engineering

9th International Work-Conference, IWBBIO 2022
Maspalomas, Gran Canaria, Spain, June 27–30, 2022
Proceedings, Part I

Springer

Editors
Ignacio Rojas
University of Granada
Granada, Spain

Fernando Rojas
ETSIIT. CITIC-UGR
University of Granada
Granada, Spain

Francisco Ortuño
University of Granada
Granada, Spain

Olga Valenzuela
Faculty of Sciences
University of Granada
Granada, Spain

Luis Javier Herrera
ETSIIT
University of Granada
Granada, Spain

ISSN 0302-9743 ISSN 1611-3349 (electronic)
Lecture Notes in Bioinformatics
ISBN 978-3-031-07703-6 ISBN 978-3-031-07704-3 (eBook)
https://doi.org/10.1007/978-3-031-07704-3

LNCS Sublibrary: SL8 – Bioinformatics

© Springer Nature Switzerland AG 2022
This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.
The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.
The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Preface

We are proud to present the final set of accepted full papers for the 9th International Work-Conference on Bioinformatics and Biomedical Engineering (IWBBIO 2022) held in Gran Canaria, Spain, during June 27–30, 2022.

IWBBIO seeks to provide a discussion forum for scientists, engineers, educators, and students about the latest ideas and realizations in the foundations, theory, models, and applications for interdisciplinary and multidisciplinary research encompassing disciplines of computer science, mathematics, statistics, biology, bioinformatics, and biomedicine.

The aim of IWBBIO 2022 was to create a friendly environment that could lead to the establishment or strengthening of scientific collaborations and exchanges among attendees, and therefore IWBBIO 2022 solicited high-quality original research papers (including significant work in progress) on any aspect of bioinformatics, biomedicine, and biomedical engineering.

Submissions relating to new computational techniques and methods in machine learning; data mining; text analysis; pattern recognition; data integration; genomics and evolution; next generation sequencing data; protein and RNA structure; protein function and proteomics; medical informatics and translational bioinformatics; computational systems biology; modeling and simulation; and their application in the life science domain, biomedicine, and biomedical engineering were especially encouraged. The list of topics in the call for papers has also evolved, resulting in the following list for the present edition:

1. **Computational proteomics**. Analysis of protein-protein interactions. Protein structure modeling. Analysis of protein functionality. Quantitative proteomics and PTMs. Clinical proteomics. Protein annotation. Data mining in proteomics.
2. **Next generation sequencing and sequence analysis**. De novo sequencing, re-sequencing, and assembly. Expression estimation. Alternative splicing discovery. Pathway analysis. Chip-seq and RNA-Seq analysis. Metagenomics. SNPs prediction.
3. **High performance in bioinformatics**. Parallelization for biomedical analysis. Biomedical and biological databases. Data mining and biological text processing. Large scale biomedical data integration. Biological and medical ontologies. Novel architecture and technologies (GPU, P2P, Grid, etc) for bioinformatics.
4. **Biomedicine**. Biomedical computing. Personalized medicine. Nanomedicine. Medical education. Collaborative medicine. Biomedical signal analysis. Biomedicine in industry and society. Electrotherapy and radiotherapy.
5. **Biomedical engineering**. E-computer-assisted surgery. Therapeutic engineering. Interactive 3D modelling. Clinical engineering. Telemedicine. Biosensors and data acquisition. Intelligent instrumentation. Patient monitoring. Biomedical robotics. Bio-nanotechnology. Genetic engineering.
6. **Computational systems for modelling biological processes**. Inference of biological networks. Machine learning in bioinformatics. Classification for

biomedical data. Microarray data analysis. Simulation and visualization of biological systems. Molecular evolution and phylogenetic modeling.
7. **Healthcare and diseases**. Computational support for clinical decisions. Image visualization and signal analysis. Disease control and diagnosis. Genome-phenome analysis. Biomarker identification. Drug design. Computational immunology.
8. **E-health**. E-health technology and devices. E-health information processing. Telemedicine/E-health application and services. Medical image processing. Video techniques for medical images. Integration of classical medicine and E-health.
9. **COVID-19**. A special session analyzing different aspects, fields of application, and technologies that have been applied against COVID-19.

After a careful peer review and evaluation process (each submission was reviewed by at least 2, and on average 3.1, Program Committee members or additional reviewers), 75 papers were accepted, according to the recommendations of reviewers and the authors' preferences, to be included in the LNBI proceedings.

IWBBIO 2022 featured several Special Sessions, which are a very useful tool in order to complement the regular program with new and emerging topics of particular interest for the participating community. Special Sessions that emphasized multidisciplinary and transversal aspects, as well as cutting-edge topics were especially encouraged and welcomed, and in this edition of IWBBIO 2022 the following were received:

– **SS1. High-throughput Genomics: Bioinformatic Tools and Medical Applications.**
Genomics is concerned with the sequencing and analysis of an organism's genome. It is involved in the understanding of how every single gene can affect the entire genome. This goal is mainly afforded using the current, cost-effective, high-throughput sequencing technologies. These technologies produce a huge amount of data that usually require high-performance computing solutions and open new ways for the study of genomics, as well as transcriptomics, gene expression, and systems biology, among others. The continuous improvements and broader applications of sequencing technologies are producing a continuous new demand for improved high-throughput bioinformatics tools.

In this context, the generation, integration, and interpretation of genetic and genomic data is driving a new era of healthcare and patient management. Medical genomics (or genomic medicine) is an emerging discipline that involves the use of genomic information about a patient as part of the clinical care with diagnostic or therapeutic purposes to improve the health outcomes. Moreover, it can be considered a subset of precision medicine that has an impact in the fields of oncology, pharmacology, rare and undiagnosed diseases, and infectious diseases. The aim of this Special Session was to bring together researchers in medicine, genomics, and bioinformatics to translate medical genomics research into new diagnostic, therapeutic, and preventive medical approaches. Therefore, we invited authors to submit original research, new tools or pipelines, and update and review articles on relevant topics, such as (but not limited to):

- Tools for data pre-processing (quality control and filtering)
- Tools for sequence mapping
- Tools for the comparison of two read libraries without an external reference
- Tools for genomic variants (such as variant calling or variant annotation)
- Tools for functional annotation: identification of domains, orthologues, genetic markers, and controlled vocabulary (GO, KEGG, InterPro, etc.)
- Tools for gene expression studies and tools for Chip-Seq data
- Integrative workflows and pipelines

Organizers: M. Gonzalo Claros, Department of Molecular Biology and Biochemistry, University of Málaga, Spain; Javier Pérez Florido, Bioinformatics Research Area, Fundación Progreso y Salud, Seville, Spain; and Francisco M. Ortuño, Department of Computer Architecture and Technology, University of Granada, Spain.

– **SS2. Feature Selection, Extraction, and Data Mining in Bioinformatics: Approaches, Methods, and Adaptations.**
Various applications of bioinformatics, system biology, and biophysics measurement data mining require proper, accurate, and precise preprocessing or data transformation before the analysis itself. Here, the most important issues are covered by the feature selection and extraction techniques to translate the raw data into the inputs for the machine learning and multivariate statistic algorithms. Even if this is a complex task, it reduces the problem dimensionality, by removing redundant or irrelevant data, without affecting significantly the principal information. The methods and approaches are often conditioned by the physical properties of the measurement process, mathematically congruent description and parameterization, and biological aspects of specific tasks. With the increasing adoption of artificial intelligence methods to solve bioinformatics problems, it is necessary to understand the conditionality of such algorithms, to choose and use the correct approach and avoid misinterpretations, artefacts, and aliasing effects. The adoption often uses existing knowledge from different fields, and direct application might underestimate the required conditions and corrupt the analysis results. This Special Session provided a forum to dicuss the multidisciplinary overlaps, development, implementation, and adoption of feature and selection methods for datasets with a biological origin in order to setup the pipeline from measurement design through signal processing to obtaining the results. The topic should cover theoretical questions, practical examples, and results verifications.

Organizer: Jan Urban, Laboratory of Signal and Image Processing, Institute of Complex Systems, South Bohemian Research Center of Aquaculture and Biodiversity of Hydrocenoses, Faculty of Fisheries and Protection of Waters, University of South Bohemia, Czech Republic.

– **SS3. Smart Healthcare Solutions for Handling COVID-19.**
Smart healthcare plays an important role towards providing robust solutions, especially for COVID-19 related problems, both locally and globally. Collection and interpretation of data worldwide and systematic research helps in identifying the potential solutions as well as predicting the future issues. This Special Session was

organized to emphasize the potential problems and the related solutions, focusing on the following topics:

- Smart wearable healthcare
- Microbiological analysis
- Minimal invasive sensors
- Biomedical waste management
- Drug-induced therapy
- Early prediction and diagnosis
- Biostatistical driven solution
- Explainable AI and deep learning driven solutions

Organizer: N. Sriraam, Department of Medical Electronics, M.S. Ramaiah Institute of Technology, India.

– **SS4. Computational Systems for Modeling of Medical Micro Sensors.**
Medical sensors are micro devices containing several parts mainly including micro-tubes, micro-valves, biological/body fluids (blood, plasma, saliva, etc.), and chemical materials (reagents and other materials). Microfluidics is an interdisciplinary field that involves the science and technology of fluid flow through systems with micro scales. Computational systems and engineering simulation are essential from the start to the end of the medical sensor design and development process. The main advantages of computational systems (AI, CFD, etc.) in medical sensors design and development are as follows:

- Improvement and optimization of design
- Acceleration in medical device innovation
- Reduction of cost and failure risk
- Reduction of production times and regulatory approval processes

The main objectives of this Special Session were as follows:

- To determine the role of computational systems (AI, CFD, etc.) in medical sensors design and development
- To determine the role of simulation in optiming the analysis process and design of medical micro-sensors
- To discuss the use of computational fluid dynamics (CFD) in analyzing medical micro sensors
- To discuss the use of computational systems to combine engineering, biology, chemical, and other criteria

Organizers: Patrizia Piro and Behrouz Pirouz, Department of Civil Engineering, University of Calabria, Italy.

It is important to note that for the sake of consistency and readability the accepted papers are organizaed into 15 chapters over two volumes, essentially following the topics

list included in the call for papers. The first volume (LNBI 13346), entitled "Bioinformatics and Biomedical Engineering. Part I" is divided into eight main parts and includes the contributions on

1. Biomedical Computing
2. Biomedical Engineering
3. Biomedical Signal Analysis
4. Biomedicine. New Advances and Applications
5. Biosensors and Data Acquisition
6. Image Visualization and Signal Analysis in Biomedical Applications
7. Computational Support for Clinical Decisions
8. COVID-19. Bioinformatics and Biomedicine

The second volume (LNBI 13347), entitled "Bioinformatics and Biomedical Engineering. Part II" is divided into seven main parts and includes the contributions on:

1. Chip-seq and RNA-Seq Analysis
2. Bioinformatics and Biomarker Identication
3. Computational Proteomics
4. Computational Systems for Modelling Biological Processes
5. Feature Selection, Extraction, and Data Mining in Bioinformatics: Approaches, Methods, and Adaptations
6. Machine Learning in Bioinformatics
7. Next Generation Sequencing and Sequence Analysis

This 9th edition of IWBBIO was organized by the University of Granada. We wish to thank our main sponsor as well as the Department of Computer Architecture and Computer Technology at the University of Granada (CITIC-UGR) and International Society for Computational Biology (ISCB) for their support and grants. We also wish to thank the editors in charge of different international journals for their interest in publishing special issues of a selection of the best papers of IWBBIO 2022. In this edition of IWBBIO there were two awards (best contribution award and best contribution from student participant) sponsored by the Editorial Office of Genes, a MDPI journal.

We would also like to express our gratitude to the members of the different committees for their support, collaboration, and good work. We especially thank the Program Committee, the reviewers, and the Special Session organizers. We also want to express our gratitude to the EasyChair platform. Finally, we wish to thank Springer for their continuous support and cooperation.

April 2022

Ignacio Rojas
Olga Valenzuela
Fernando Rojas
Luis Javier Herrera
Francisco Ortuño

Organization

Conference Chairs

Ignacio Rojas	University of Granada, Spain
Olga Valenzuela	University of Granada, Spain
Fernando Rojas	University of Granada, Spain
Luis Javier Herrera	University of Granada, Spain
Francisco Ortuño	University of Granada, Spain

Steering Committee

Miguel A. Andrade	University of Mainz, Germany
Hesham H. Ali	University of Nebraska, USA
Oresti Baños	University of Granada, Spain
Alfredo Benso	Politecnico di Torino, Italy
Larbi Boubchir	LIASD, University of Paris 8, France
Giorgio Buttazzo	Superior School Sant'Anna, Italy
Gabriel Caffarena	University San Pablo CEU, Spain
Mario Cannataro	Magna Graecia University of Catanzaro, Italy
Jose María Carazo	Spanish National Center for Biotechnology (CNB), Spain
Jose M. Cecilia	Universidad Católica San Antonio de Murcia (UCAM), Spain
M. Gonzalo Claros	University of Malaga, Spain
Joaquin Dopazo	Fundacion Progreso y Salud, Spain
Werner Dubitzky	University of Ulster, UK
Afshin Fassihi	Universidad Católica San Antonio de Murcia (UCAM), Spain
Jean-Fred Fontaine	University of Mainz, Germany
Humberto Gonzalez	University of Basque Country (UPV/EHU), Spain
Concettina Guerra	Georgia Tech, USA
Roderic Guigo	Pompeu Fabra University, Spain
Andy Jenkinson	Karolinska Institute, Sweden
Craig E. Kapfer	Reutlingen University, Germany
Narsis Aftab Kiani	European Bioinformatics Institute (EBI), UK
Natividad Martinez	Reutlingen University, Germany
Marco Masseroli	Politechnical University of Milan, Italy
Federico Moran	Complutense University of Madrid, Spain

Cristian R. Munteanu	University of A Coruña, Spain
Jorge A. Naranjo	NYU Abu Dhabi, Abu Dhabi
Michael Ng	Hong Kong Baptist University, China
Jose L. Oliver	University of Granada, Spain
Juan Antonio Ortega	University of Seville, Spain
Fernando Rojas	University of Granada, Spain
Alejandro Pazos	University of A Coruña, Spain
Javier Perez Florido	Genomics and Bioinformatics Platform of Andalusia, Spain
Violeta I. Pérez Nueno	Inria Nancy-Grand Est and Loria, France
Horacio Pérez-Sánchez	Universidad Católica San Antonio de Murcia (UCAM), Spain
Alberto Policriti	Università di Udine, Italy
Omer F. Rana	Cardiff University, UK
M. Francesca Romano	Superior School Sant'Anna, Italy
Yvan Saeys	Ghent University, Belgium
Vicky Schneider	The Genome Analysis Centre (TGAC), UK
Ralf Seepold	HTWG Konstanz, Germany
Mohammad Soruri	University of Birjand, Iran
Yoshiyuki Suzuki	Tokyo Metropolitan Institute of Medical Science, Japan
Oswaldo Trelles	University of Malaga, Spain
Shusaku Tsumoto	Shimane University, Japan
Renato Umeton	Dana-Farber Cancer Institute and Massachusetts Institute of Technology, USA
Jan Urban	University of South Bohemia, Czech Republic
Alfredo Vellido	Polytechnic University of Catalonia, Spain
Wolfgang Wurst	GSF National Research Center of Environment and Health, Germany

Program Committee and Additional Reviewers

Magda Abdellattif	Taif University, Saudi Arabia
Fares Al-Shargie	American University of Sharjah, United Arab Emirates
Jesus Alcala-Fdez	University of Granada, Spain
Hesham Ali	University of Nebraska Omaha, USA
Georgios Anagnostopoulos	Florida Institute of Technology, USA
Patrizio Arrigo	SCITEC, Italy
Gajendra Kumar Azad	Patna University, India
Hazem Bahig	Ain Shams University, Egypt
Ugo Bastolla	Centro de Biologia Molecular Severo Ochoa, Spain

Payam Behzadi	Islamic Azad University, Iran
Alfredo Benso	Politecnico di Torino, Italy
Anna Bernasconi	Politecnico di Milano, Italy
Mahua Bhattacharya	Indian Institute of Information Technology and Management, Gwalior, India
Paola Bonizzoni	Università di Milano-Bicocca, Italy
Larbi Boubchir	University of Paris 8, France
Hacene Boukari	Delaware State University, USA
Gabriel Caffarena	Universidad CEU San Pablo, Spain
Mario Cannataro	Magna Graecia University of Catanzaro, Italy
Jose Maria Carazo	National Center for Biotechnology (CNB-CSIC), Spain
Rita Casadio	University of Bologna, Italy
Daniel Castillo-Secilla	University of Granada, Spain
Claudia Cava	IBFM-CNR, Italy
Francisco Cavas-Martínez	Technical University of Cartagena, Spain
Chinmay Chakraborty	Birla Institute of Technology, India
Ting-Fung Chan	The Chinese University of Hong Kong, Hong Kong
Satyendra Chandra Tripathi	AIIMS Nagpur, India
Kun-Mao Chao	National Taiwan University, Taiwan
Bolin Chen	Northwestern Polytechnical University, China
Brian Chen	Lehigh University, USA
Chuming Chen	University of Delaware, USA
Jeonghyeon Choi	Georgia Regents University, USA
Javier Cifuentes Faura	University of Murcia, Spain
M. Gonzalo Claros	Universidad de Málaga, Spain
Zhu Daming	Shandong University, China
Bhaskar Dasgupta	University of Illinois at Chicago, USA
Alexandre G. De Brevern	INSERM UMR-S, Université Paris Cité, France
Javier De Las Rivas	Cancer Research Center (CiC-IBMCC, CSIC/USAL/IBSAL), Spain
Ricardo de Matos Simoes	Harvard University, USA
Marie-Dominique Devignes	Loria, France
Paolo Di Giamberardino	Sapienza University of Rome, Italy
Maria Natalia Dias Soeiro Cordeiro	University of Porto, Portugal
Marko Djordjevic	University of Belgrade, Serbia
Joaquin Dopazo	Fundacion Progreso y Salud, Spain
Mohammed Elmogy	Mansoura University, Egypt
Gionata Fragomeni	Magna Graecia University of Catanzaro, Italy
Hassan Ghazal	Mohammed I University, Morocco

Razvan Ghinea	University of Granada, Spain
Christophe Guyeux	University of Franche-Comté, France
Pietro Hiram Guzzi	Magna Graecia University of Catanzaro, Italy
Michael Hackenberg	University of Granada, Spain
Nurit Haspel	University of Massachusetts Boston, USA
Morihiro Hayashida	National Institute of Technology, Matsue College, Japan
Luis Herrera	University of Granada, Spain
Ralf Hofestaedt	Bielefeld University, Germany
Jingshan Huang	University of South Alabama, USA
Cosimo Ieracitano	University Mediterranea of Reggio Calabria, Italy
Chang-Hwan Im	Hanyang University, South Korea
Hamed Khodadadi	Islamic Azad University, Iran
Narsis Kiani	Karolinska Institute, Sweden
Tomas Koutny	University of West Bohemia, Czech Republic
Konstantin Krutovsky	Georg-August-University of Göttingen, Germany
Chen Li	Monash University, Australia
Shuai Cheng Li	City University of Hong Kong, Hong Kong
Li Liao	University of Delaware, USA
Hongfei Lin	Dalian University of Technology, China
Javier Martin	IPBLN-CSIC, Spain
Francisco Martínez-Álvarez	Universidad Pablo de Olavide, Spain
Roderick Melnik	Wilfrid Laurier University, Canada
Francesco Carlo Morabito	University of Reggio Calabria, Italy
Enrique Muro	Johannes Gutenberg University, Germany
Kenta Nakai	University of Tokyo, Japan
Isabel Nepomuceno	University of Seville, Spain
Dang Ngoc Hoang Thanh	University of Economics Ho Chi Minh City, Vietnam
José Luis Oliveira	University of Aveiro, Portugal
Yuriy Orlov	Institute of Cytology and Genetics, Russia
Juan Antonio Ortega	University of Seville, Spain
Andres Ortiz	University of Malaga, Spain
Francisco Manuel Ortuño	University of Granada, Spain
Motonori Ota	Nagoya University, Japan
Mehmet Akif Ozdemir	Izmir Katip Celebi University, Turkey
Joel P. Arrais	University of Coimbra, Portugal
Paolo Paradisi	ISTI-CNR, Italy
Taesung Park	Seoul National University, South Korea
Antonio Pinti	I3MTO Orléans, France
Yuri Pirola	Università degli Studi di Milano-Bicocca, Italy
Joanna Polanska	The Silesian University of Technology, Poland

Alberto Policriti	University of Udine, Italy
Hector Pomares	University of Granada, Spain
María M. Pérez	University of Granada, Spain
Hossein Rabbani	Isfahan University of Medical Sciences, Iran
Amgad Rabie	Ain Shams University, Egypt
Jiulietta Rau	Istituto di Struttura della Materia, Italy
Khalid Raza	Jamia Millia Islamia, India
Jairo Rocha	University of the Balearic Islands, Spain
Maria Rodriguez Martinez	IBM Zurich Research Laboratory, Switzerland
Fernando Rojas	University of Granada, Spain
Ignacio Rojas	University of Granada, Spain
Gregorio Rubio	Universitat Politècnica de València, Spain
Irena Rusu	LINA, University of Nantes, France
Michael Sadovsky	Institute of Computational Modelling of SB RAS, Russia
Beata Sarecka-Hujar	Medical University of Silesia in Katowice, Poland
Jean-Marc Schwartz	University of Manchester, UK
Russell Schwartz	Carnegie Mellon University, USA
Preeti Singh	UIET, India
Surinder Singh	Panjab University, India
Sónia Sobral	Universidade Portucalense, Portugal
Jiangning Song	Monash University, Australia
Joe Song	New Mexico State University, USA
Natarajan Sriraam	M.S. Ramaiah Institute of Technology, India
Jiangtao Sun	Beihang University, China
Wing-Kin Sung	National University of Singapore, Singapore
Prashanth Suravajhala	Amrita University Kerala, India
Martin Swain	Aberystwyth University, UK
Sing-Hoi Sze	Texas A&M University, USA
Alessandro Tonacci	IFC-CNR, Italy
Carolina Torres	University of Granada, Spain
Marcos Roberto Tovani Palone	University of São Paulo, Brazil
Shusaku Tsumoto	Shimane University, Japan
Renato Umeton	Massachusetts Institute of Technology, USA
Jan Urban	Institute of Complex Systems, FFPW USB, Czech Republic
Olga Valenzuela	University of Granada, Spain
Alfredo Vellido	Universitat Politècnica de Catalunya, Spain
Jianxin Wang	Central South University, China
Jiayin Wang	Xi'an Jiaotong University, China
Junbai Wang	Radium Hospital, Norway
Lusheng Wang	City University of Hong Kong, Hong Kong

Ka-Chun Wong	City University of Hong Kong, Hong Kong
Phil Yang	George Mason University, USA
Jin Zhang	Washington University in St. Louis, USA
Yudong Zhang	University of Leicester, UK
Zhongming Zhao	University of Texas Health Science Center at Houston, USA
Huiru Zheng	University of Ulster, UK
Shanfeng Zhu	Fudan University, China

Contents – Part I

Biomedical Computing

Calculation of DNA Strand Breaks by Types of Electron Interaction with Monte Carlo Simulation 3
Youssef Lamghari, Huizhong Lu, and M'hamed Bentourkia

Linear Predictive Modeling for Immune Metabolites Related to Other Metabolites 16
Jana Schwarzerova, Iro Pierides, Karel Sedlar, and Wolfram Weckwerth

Modelling of Arbitrary Shaped Channels and Obstacles by Distance Function 28
Kristína Kovalčíková Ďuračíková, Alžbeta Bugáňová, and Ivan Cimrák

Gene Expression Profiles of Visceral and Subcutaneous Adipose Tissues in Children with Overweight or Obesity: The KIDADIPOSEQ Project 42
Mireia Bustos-Aibar, Augusto Anguita-Ruiz, Álvaro Torres-Martos, Jesús Alcalá-Fdez, Francisco Javier Ruiz-Ojeda, Marjorie Reyes-Farias, Andrea Soria-Gondek, Laura Herrero, David Sánchez-Infantes, and Concepción María Aguilera

The Role of Astrocytes in Alzheimer's Disease Progression 47
Swadesh Pal and Roderick Melnik

Effects of Random Inputs and Short-Term Synaptic Plasticity in a LIF Conductance Model for Working Memory Applications 59
Thi Kim Thoa Thieu and Roderick Melnik

Biomedical Engineering

Thermal Effects of Manual Therapy in Low Back Pain: A Pilot Study 75
Andrea Rosales-Hernandez, Daniela Vigueras-Becerril, Arely G. Morales-Hernandez, Sandra M. Chavez-Monjaras, Luis A. Morales-Hernandez, and Irving A. Cruz-Albarran

Bone Health Parameters in Young Adult Female Handball Players 90
Elie Maliha, Anthony Khawaja, Hechmi Toumi, Rachid Jennane, Antonio Pinti, and Rawad El Hage

Adaptative Modelling of the Corneal Architecture in a Free-of-Stress State in Incipient Keratoconus 108
Francisco Cavas, Carmelo Gómez, José S. Velázquez, David Piñero, Francisco L. Sáez-Gutiérrez, and Jorge Alió

Design of an Analysis Method for the Human Cornea's Bilateral Symmetry. A Case-Study in Healthy Patients 119
Francisco Cavas, José S. Velázquez, Carmelo Gómez, Jorge Mira, Francisco L. Sáez-Gutiérrez, and Jorge Alió

Biomedical Signal Analysis

Automated TTC Image-Based Analysis of Mouse Brain Lesions 135
Gerasimos Damigos, Nefeli Zerva, Angelos Pavlopoulos, Konstantina Chatzikyrkou, Argyro Koumenti, Konstantinos Moustakas, Constantinos Pantos, Iordanis Mourouzis, Athanasios Lourbopoulos, and Evangelia I. Zacharaki

PET-Neuroimaging and Neuropsychological Study for Early Cognitive Impairment in Parkinson's Disease 143
Sergey Lytaev

Architecture and Calibration of a Multi-channel Electrical Impedance Myographer 154
Edson Rodrigues, Erick Dario León Bueno de Camargo, and Olavo Luppi Silva

Biomedicine. New Advances and Applications

Advanced Incremental Attribute Learning Clustering Algorithm for Medical and Healthcare Applications 171
Siwar Gorrab, Fahmi Ben Rejab, and Kaouther Nouira

Assessment of Inflammation in Non-calcified Artery Plaques with Dynamic 18F-FDG-PET/CT: CT Alone, Does-It Detect the Vulnerable Plaque? 184
Mamdouh S. Al-enezi, Abdelouahed Khalil, Tamas Fulop, Éric Turcotte, and M'hamed Bentourkia

Comparative Analysis of the Spatial Structure Chloroplasts and Cyanobacteria Photosynthetic Systems I and II Genes 197
Maria Senashova and Michael Sadovsky

Unsupervised Classification of Some Bacteria with 16S RNA Genes 205
Agnia Teterleva, Vladislav Abramov, Andrey Morgun, Irina Larionova, and Michael Sadovsky

Modern Approaches to Cancer Treatment 216
Snezhana M. Bakalova, Milena Georgieva, and Jose Kaneti

A Service for Flexible Management and Analysis of Heterogeneous Clinical Data 227
Sandro Hurtado, José García-Nieto, and Ismael Navas-Delgado

Biosensors and Data Acquisition

Reconfigurable Arduino Shield for Biosignal Acquisition 241
Leozítor Floro de Souza, Fábio Iaione, and Shih Ting Ju

Smart Watch for Smart Health Monitoring: A Literature Review 256
Avnish Singh Jat and Tor-Morten Grønli

Data Quality Enhancement for Machine Learning on Wearable ECGs 269
Balázs Molnár, László Micsinyei, Gábor Perlaki, Gergely Orsi, László Hejjel, Tamás Dóczi, József Janszky, Norbert Laky, and Ákos Tényi

Image Visualization and Signal Analysis in Biomedical Applications

Measurable Difference Between Malignant and Benign Tumor of the Thyroid Gland Recognizable Using Echogenicity Index in Ultrasound B-MODE Imaging: An Experimental Blind Study 283
Jiri Blahuta, Tomas Soukup, Jan Lavrincik, Lukas Pavlik, and Zuzana Repaska

Initial Prototype of Low-Cost Stool Monitoring System for Early Detection of Diseases 297
José Luis López-Ruiz, David Díaz-Jiménez, Alicia Montoro-Lendínez, and Macarena Espinilla

Cerebral Activation in Subjects with Developmental Coordination Disorder: A Pilot Study with PET Imaging 309
Marie Farmer, Bernard Echenne, and M'hamed Bentourkia

On the Use of Explainable Artificial Intelligence for the Differential Diagnosis of Pigmented Skin Lesions 319
Sandro Hurtado, Hossein Nematzadeh, José García-Nieto, Miguel-Ángel Berciano-Guerrero, and Ismael Navas-Delgado

Estimating Frontal Body Landmarks from Thermal Sensors Using Residual Neural Networks 330
Aurora Polo-Rodríguez, Marcos Lupión, Pilar M. Ortigosa, and Javier Medina-Quero

NMF for Quality Control of Multi-modal Retinal Images for Diagnosis of Diabetes Mellitus and Diabetic Retinopathy 343
Anass Benali, Laura Carrera, Ann Christin, Ruben Martín, Anibal Alé, Marina Barraso, Carolina Bernal, Sara Marín, Silvia Feu, Josep Rosinés, Teresa Hernandez, Irene Vilá, Cristian Oliva, Irene Vinagre, Emilio Ortega, Marga Gimenez, Enric Esmatjes, Javier Zarranz-Ventura, Enrique Romero, and Alfredo Vellido

Radiomic-Based Lung Nodule Classification in Low-Dose Computed Tomography 357
Wojciech Prazuch, Malgorzata Jelitto-Gorska, Agata Durawa, Katarzyna Dziadziuszko, and Joanna Polanska

Segmentation of Brain MR Images Using Quantum Inspired Firefly Algorithm with Mutation 364
Alokeparna Choudhury, Sourav Samanta, Sanjoy Pratihar, and Oishila Bandyopadhyay

Computational Support for Clinical Decisions

Single-Channel EEG Detection of REM Sleep Behaviour Disorder: The Influence of REM and Slow Wave Sleep 381
Irene Rechichi, Federica Amato, Alessandro Cicolin, and Gabriella Olmo

A Deep Learning Framework for the Prediction of Conversion to Alzheimer Disease 395
Sofia Ostellino, Alfredo Benso, and Gianfranco Politano

Gene Expression Tools from a Technical Perspective: Current Approaches and Alternative Solutions for the KnowSeq Suite 404
Daniel Castillo-Secilla, Daniel Redondo-Sánchez, Luis Javier Herrera, Ignacio Rojas, and Alberto Guillén

COVID-19. Bioinformatics and Biomedicine

Optimal Chair Location Through a Maximum Diversity Problem Genetic Algorithm Optimization 417
Rubén Ferrero-Guillén, Javier Díez-González, Paula Verde, Alberto Martínez-Gutiérrez, José-Manuel Alija-Pérez, and Rubén Álvarez

Collecting SARS-CoV-2 Encoded miRNAs via Text Mining 429
Alexandra Schubö, Armin Hadziahmetovic, Markus Joppich, and Ralf Zimmer

COVID-19 Severity Classification Using a Hierarchical Classification Deep Learning Model 442
Sergio Ortiz, Juan Carlos Morales, Fernando Rojas, Olga Valenzuela, Luis Javier Herrera, and Ignacio Rojas

The Role of Information Sources, Trust in Information Sources, and COVID-19 Conspiracy Theory in the Compliance with COVID-19 Related Measures 453
Ana Jovančević, Izabel Cvetković, and Nebojša Milićević

Author Index 459

Contents – Part II

Chip-Seq and RNA-Seq Analysis

Integrative Analysis of Ovarian Serious Adenocarcinoma to Understand Disease Network Biology 3
Sahar Qazi and Khalid Raza

GAGAM: A Genomic Annotation-Based Enrichment of scATAC-seq Data for Gene Activity Matrix 18
Lorenzo Martini, Roberta Bardini, Alessandro Savino, and Stefano Di Carlo

Finding Significantly Enriched Cells in Single-Cell RNA Sequencing by Single-Sample Approaches 33
Anna Mrukwa, Michal Marczyk, and Joanna Zyla

Comparison of Stranded and Non-stranded RNA-Seq in Predicting Small RNAs in a Non-model Bacterium 45
Karel Sedlar and Ralf Zimmer

Comparative Study of Synthetic Bulk RNA-Seq Generators 57
Felitsiya Shakola, Dean Palejev, and Ivan Ivanov

Investigating Sources of Zeros in 10× Single-Cell RNAseq Data 71
Hanna Slowik, Joanna Zyla, and Michal Marczyk

Bioinformatics and Biomarker Identification

Exhaled Breath Condensate Study for Biomarkers Discovery 83
S. Patsiris, T. Exarchos, and P. Vlamos

Statistical Learning Analysis of Thyroid Cancer Microarray Data 90
Iván Petrini, Rocío L. Cecchini, Marilina Mascaró, Ignacio Ponzoni, and Jessica A. Carballido

Migrating CUDA to oneAPI: A Smith-Waterman Case Study 103
Manuel Costanzo, Enzo Rucci, Carlos García-Sánchez, Marcelo Naiouf, and Manuel Prieto-Matías

Computational Proteomics

Fuzzy-Inference System for Isotopic Envelope Identification in Mass Spectrometry Imaging Data 119
Anna Glodek

Receptor Tyrosine Kinase KIT: A New Look for an Old Receptor 133
Julie Ledoux and Luba Tchertanov

Human Vitamin K Epoxide Reductase as a Target of Its Redox Protein 138
Julie Ledoux, Maxim Stolyarchuk, and Luba Tchertanov

A Distance Geometry Procedure Using the Levenberg-Marquardt Algorithm and with Applications in Biology but Not only 142
Douglas S. Gonçalves and Antonio Mucherino

A Semi-supervised Graph Deep Neural Network for Automatic Protein Function Annotation 153
Akrem Sellami, Bishnu Sarker, Salvatore Tabbone, Marie-Dominique Devignes, and Sabeur Aridhi

Computational Systems for Modelling Biological Processes

Strong Prevalence of the Function over Taxonomy in Human *t*RNA Genes 169
Yana Nedorez and Michael Sadovsky

A Methodology for Co-simulation-Based Optimization of Biofabrication Protocols 179
Leonardo Giannantoni, Roberta Bardini, and Stefano Di Carlo

A 3D Multicellular Simulation Layer for the Synthetic Biology CAD Infobiotics Workbench Suite 193
Richard Oliver Matzko, Laurentiu Mierla, and Savas Konur

Integrating *in-vivo* Data in CFD Simulations and in *in-vitro* Experiments of the Hemodynamic in Healthy and Pathologic Thoracic Aorta 208
Alessandro Mariotti, Emanuele Gasparotti, Emanuele Vignali, Pietro Marchese, Simona Celi, and Maria Vittoria Salvetti

Sensitivity Analysis of Adhesion in Computational Model of Elastic Doublet 220
Alžbeta Bohiniková, Iveta Jančigová, Ivan Cimrák, and James J. Feng

Increasing the Accuracy of Optipharm's Virtual Screening Predictions by Implementing Molecular Flexibility 234
Savíns Puertas-Martín, Juana L. Redondo, Ester M. Garzón, Horacio Pérez-Sánchez, and Pilar M. Ortigosa

Feature Selection, Extraction, and Data Mining in Bioinformatics: Approaches, Methods and Adaptations

Comparisons of Knowledge Graphs and Entity Extraction in Breast Cancer Subtyping Biomedical Text Analysis 249
Jean Davidson, Grif Hawblitzel, McClain Kressman, Andrew Doud, Harsha Lakshmankumar, Ella Thomas, Paul Kim, Ava Jakusovszky, and Paul Anderson

Towards XAI: Interpretable Shallow Neural Network Used to Model HCP's fMRI Motor Paradigm Data 260
José Diogo Marques dos Santos and José Paulo Marques dos Santos

A Deep Learning-Based Method for Uncovering GPCR Ligand-Induced Conformational States Using Interpretability Techniques 275
Mario A. Gutiérrez-Mondragón, Caroline König, and Alfredo Vellido

Data Transformation for Clustering Utilization for Feature Detection in Mass Spectrometry 288
Vojtech Barton and Helena Skutkova

Spolmap: An Enriched Visualization of CRISPR Diversity 300
Christophe Guyeux, Guislaine Refrégier, and Christophe Sola

How to Compare Various Clustering Outcomes? Metrices to Investigate Breast Cancer Patient Subpopulations Based on Proteomic Profiles 309
Joanna Tobiasz and Joanna Polanska

Sperm-cell Detection Using YOLOv5 Architecture 319
Michal Dobrovolny, Jakub Benes, Ondrej Krejcar, and Ali Selamat

Machine Learning in Bioinformatics

Comparative Analysis of Supervised Cell Type Detection in Single-Cell RNA-seq Data 333
Akram Vasighizaker, Sheena Hora, Yash Trivedi, and Luis Rueda

PathWeigh – Quantifying the Behavior of Biochemical Pathway Cascades 346
Dani Livne and Sol Efroni

Translational Challenges of Biomedical Machine Learning Solutions in Clinical and Laboratory Settings 353
Carlos Vega, Miroslav Kratochvil, Venkata Satagopam, and Reinhard Schneider

Human Multi-omics Data Pre-processing for Predictive Purposes Using Machine Learning: A Case Study in Childhood Obesity 359
Álvaro Torres-Martos, Augusto Anguita-Ruiz, Mireia Bustos-Aibar, Sofia Cámara-Sánchez, Rafael Alcalá, Concepción M. Aguilera, and Jesús Alcalá-Fdez

Feature Density as an Uncertainty Estimator Method in the Binary Classification Mammography Images Task for a Supervised Deep Learning Model 375
Ricardo Javier Fuentes-Fino, Saúl Calderón-Ramírez, Enrique Domínguez, Ezequiel López-Rubio, Marco A. Hernandez-Vasquez, and Miguel A. Molina-Cabello

Iterative Clustering for Differential Gene Expression Analysis 389
Olga Georgieva

Comparison of Batch Effect Removal Methods for High Dimensional Mass Cytometry Data 399
Aleksandra Suwalska, Nelita du Plessis-Burger, Gian van der Spuy, and Joanna Polanska

Next Generation Sequencing and Sequence Analysis

Evaluating Performance of Regression and Classification Models Using Known Lung Carcinomas Prognostic Markers 413
Shrikant Pawar, Karuna Mittal, and Chandrajit Lahiri

Approximate Pattern Matching Using Search Schemes and In-Text Verification 419
Luca Renders, Lore Depuydt, and Jan Fostier

KFinger: Capturing Overlaps Between Long Reads by Using Lyndon Fingerprints 436
Paola Bonizzoni, Alessia Petescia, Yuri Pirola, Raffaella Rizzi, Rocco Zaccagnino, and Rosalba Zizza

Can We Detect T Cell Receptors from Long-Read RNA-Seq Data? 450
Justyna Mika, Serge M. Candéias, Christophe Badie, and Joanna Polanska

Author Index 465