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Bioinformatics and Biomedical Engineering

7th International Work-Conference, IWBBIO 2019
Granada, Spain, May 8–10, 2019
Proceedings, Part I

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Preface

We are proud to present the set of final accepted full papers for the 7th edition of the IWBBIO conference—International Work-Conference on Bioinformatics and Biomedical Engineering—held in Granada (Spain) during May 8–10, 2019.

IWBBIO 2019 sought 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 aims of IWBBIO are to create a friendly environment that could lead to the establishment or strengthening of scientific collaborations and exchanges among attendees, and therefore IWBBIO 2019 solicited high-quality original research papers (including significant work-in-progress) on any aspect of bioinformatics, biomedicine, and biomedical engineering.

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 successive 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.** Computer-assisted surgery; therapeutic engineering; interactive 3D modeling; clinical engineering; telemedicine; biosensors and data acquisition; intelligent instrumentation; patient monitoring; biomedical robotics; bio-nanotechnology; genetic engineering.
6. **Computational systems for modeling 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. **Health care 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.

After a careful peer review and evaluation process (each submission was reviewed by at least two, and on average 3.2, Program Committee members or additional reviewer), 97 papers were accepted for oral, poster, or virtual presentation, according to the recommendations of reviewers and the authors' preferences, and to be included in the LNBI proceedings.

During IWBBIO 2019 several special sessions were held. Special sessions are a very useful tool to complement the regular program with new and emerging topics of particular interest for the participating community. Special sessions that emphasize multi-disciplinary and transversal aspects, as well as cutting-edge topics, are especially encouraged and welcome, and in this edition of IWBBIO they were the following:

– **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 opens new ways for the study of genomics, but also transcriptomics, gene expression, and systems biology, among others. The continuous improvements and broader applications on sequencing technologies is generating a continuous new demand of improved high-throughput bioinformatics tools. Genomics is concerned with the sequencing and analysis of an organism genome taking advantage of the current, cost-effective, high-throughput sequencing technologies. Continuous improvement of genomics is in turn leading to a continuous new demand of enhanced high-throughput bioinformatics tools. In this context, the generation, integration, and interpretation of genetic and genomic data are driving a new era of health-care and patient management. Medical genomics (or genomic medicine) is this 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 is having an impact in the fields of oncology, pharmacology, rare and undiagnosed diseases, and infectious diseases. The aim of this special session is to bring together researchers in medicine, genomics, and bioinformatics to translate medical genomics research into new diagnostic, therapeutic, and preventive medical approaches. Therefore, we invite authors to submit original research, new tools or

pipelines, or their 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, orthologs, genetic markers, controlled vocabulary (GO, KEGG, InterPro, etc.)
- Tools for gene expression studies
- Tools for Chip-Seq data
- Integrative workflows and pipelines

Organizers: Prof. M. Gonzalo Claros, Department of Molecular Biology and Biochemistry, University of Málaga, Spain

Dr. Javier Pérez Florido, Bioinformatics Research Area, Fundación Progreso y Salud, Seville, Spain

Dr. Francisco M. Ortuño, Bioinformatics Research Area, Fundación Progreso y Salud, Seville, Spain

– SS2. Omics Data Acquisition, Processing, and Analysis

Automation and intelligent measurement devices produce multiparametric and structured huge datasets. The incorporation of the multivariate data analysis, artificial intelligence, neural networks, and agent-based modeling exceeds the experiences of classic straightforward evaluation and reveals emergent attributes, dependences, or relations. For the wide spectrum of techniques, genomics, transcriptomics, metabolomics, proteomics, lipidomics, aquaphotomics, etc., the superposition of expert knowledge from bioinformatics, biophysics, and biocybernetics is required. The series of systematic experiments have to also deal with the data pipelines, databases, sharing, and proper description. The integrated concepts offer robust evaluation, verification, and comparison.

In this special section a discussion on novel approaches in measurement, algorithms, methods, software, and data management focused on the omic sciences is provided. The topic covers practical examples, strong results, and future visions.

Organizer: Dipl-Ing. Jan Urban, PhD, Head of laboratory of signal and image processing. University of South Bohemia in České Budejovice, Faculty of Fisheries and Protection of Waters, South Bohemian Research Center of Aquaculture and Biodiversity of Hydrocenoses, Institute of Complex Systems, Czech Republic.

Websites:

www.frov.jcu.cz/en/institute-complex-systems/lab-signal-image-processing

– SS3. Remote Access, Internet of Things, and Cloud Solutions for Bioinformatics and Biomonitoring

The current process of the 4th industrial revolution also affects bioinformatic data acquisition, evaluation, and availability. The novel cyberphysical measuring

devices are smart, autonomous, and controlled online. Cloud computing covers data storage and processing, using artificial intelligence methods, thanks to massive computational power. Laboratory and medical practice should be on the apex of developing, implementing, and testing the novel bioinformatic approaches, techniques, and methods, so as to produce excellent research results and increase our knowledge in the field.

In this special section, results, concepts, and ongoing research with novel approaches to bioinformatics, using the Internet of Things (IoT) devices is presented.

Organizer: Antonin Barta, Antonin Barta, Faculty of Fishery and Waters Protection, Czech Republic

– **SS4: Bioinformatics Approaches for Analyzing Cancer Sequencing Data**

In recent years, next-generation sequencing has enabled us to interrogate entire genomes, exomes, and transcriptomes of tumor samples and to obtain high-resolution landscapes of genetic changes at the single-nucleotide level. More and more novel methods are proposed for efficient and effective analyses of cancer sequencing data. One of the most important questions in cancer genomics is to differentiate the patterns of the somatic mutational events. Somatic mutations, especially the somatic driver events, are considered to govern the dynamics of clone birth, evolution, and proliferation. Recent studies based on cancer sequencing data, across a diversity of solid and hematological disorders, have reported that tumor samples are usually both spatially and temporally heterogeneous and frequently comprise one or multiple founding clone(s) and a couple of sub-clones. However, there are still several open problems in cancer clonality research, which include (1) the identification of clonality-related genetic alterations, (2) discerning clonal architecture, (3) understanding their phylogenetic relationships, and (4) modeling the mathematical and physical mechanisms. Strictly speaking, none of these issues is completely solved, and these issues remain in the active areas of research, where powerful and efficient bioinformatics tools are urgently demanded for better analysis of rapidly accumulating data. This special issue aims to publish the novel mathematical and computational approaches and data processing pipelines for cancer sequencing data, with a focus on those for tumor micro-environment and clonal architecture.

Organizers: Jiayin Wang, PhD, Professor, Jiayin Wang, PhD, Professor, Department of Computer Science and Technology, Xian Jiaotong University, China

Xuanping Zhang, PhD, Associate Professor, Xuanping Zhang, PhD, Associate Professor, Department of Computer Science and Technology, Xian Jiaotong University, China.

Zhongmeng Zhao, PhD, Professor, Zhongmeng Zhao, PhD, Professor, Department of Computer Science and Technology, Xian Jiaotong University, China

– **SS5. Telemedicine for Smart Homes and Remote Monitoring**

Telemedicine in smart homes and remote monitoring is implementing a core research to link up devices and technologies from medicine and informatics. A person's vital data can be collected in a smart home environment and transferred to medical databases and the professionals. Most often different from clinical approaches, key instruments are specifically tailored devices, multidevices, or even wearable devices respecting always individual preferences and non-intrusive paradigms. The proposed session focused on leading research approaches, prototypes, and implemented hardware/software co-designed systems with a clear networking applicability in smart homes with unsupervised scenarios.

Organizers: Prof. Dr. Juan Antonio Ortega. Director of the Centre of Computer Scientific in Andalusia, Spain, Head of Research Group IDINFOR (TIC223), University of Seville, ETS Ingeniería Informática, Spain

Prof. Dr. Natividad Martínez Madrid. Head of the Internet of Things Laboratory and Director of the AAL-Living Lab at Reutlingen University, Department of Computer Science, Reutlingen, Germany

Prof. Dr. Ralf Seepold. Head of the Ubiquitous Computing Lab at HTWG Konstanz, Department of Computer Science, Konstanz, Germany

– **SS6. Clustering and Analysis of Biological Sequences with Optimization Algorithms**

The analysis of DNA sequences is a crucial application area in computational biology. Finding similarity between genes and DNA subsequences provides very important knowledge of their structures and their functions. Clustering as a widely used data mining approach has been carried out to discover similarity between biological sequences. For example, by clustering genes, their functions can be predicted according to the known functions of other genes in the similar clusters. The problem of clustering sequential data can be solved by several standard pattern recognition techniques such as k-means, k-nearest neighbors, and the neural networks. However, these algorithms become very complex when observations are sequences with variable lengths, like genes. New optimization algorithms have shown that they can be successfully utilized for biological sequence clustering.

Organizers: Prof. Dr. Mohammad Soruri Faculty of Electrical and Computer Engineering, University of Birjand, Birjand, Iran. Ferdows Faculty of Engineering, University of Birjand, Birjand, Iran

– **SS7. Computational Approaches for Drug Repurposing and Personalized Medicine**

With continuous advancements of biomedical instruments and the associated ability to collect diverse types of valuable biological data, numerous recent research studies have been focusing on how to best extract useful information from the ‘big biomedical data’ currently available. While drug design has been one of the most essential areas of biomedical research, the drug design process for the most part has not fully benefited from the recent explosion in the growth of biological data and bioinformatics algorithms. With the incredible overhead associated with the traditional drug design process in terms of time and cost, new alternative methods, possibly based on computational approaches, are very much needed to propose innovative ways for effective drugs and new treatment options. As a result, drug repositioning or repurposing has gained significant attention from biomedical researchers and pharmaceutical companies as an exciting new alternative for drug discovery that benefits from the computational approaches. This new development also promises to transform health care to focus more on individualized treatments, precision medicine, and lower risks of harmful side effects. Other alternative drug design approaches that are based on analytical tools include the use of medicinal natural plants and herbs as well as using genetic data for developing multi-target drugs.

Organizer: Prof. Dr. Hesham H. Ali, UNO Bioinformatics Core Facility College of Information Science and Technology University of Nebraska at Omaha, USA

It is important to note, that for the sake of consistency and readability of the book, the presented papers are classified under 14 chapters. The organization of the papers is in two volumes arranged basically following the topics list included in the call for papers. The first volume (LNBI 11465), entitled “Bioinformatics and Biomedical Engineering. Part I,” is divided into eight main parts and includes contributions on:

1. High-throughput genomics: bioinformatic tools and medical applications
2. Omics data acquisition, processing, and analysis
3. Bioinformatics approaches for analyzing cancer sequencing data
4. Next-generation sequencing and sequence analysis
5. Structural bioinformatics and function
6. Telemedicine for smart homes and remote monitoring
7. Clustering and analysis of biological sequences with optimization algorithms
8. Computational approaches for drug repurposing and personalized medicine

The second volume (LNBI 11466), entitled “Bioinformatics and Biomedical Engineering. Part II,” is divided into six main parts and includes contributions on:

1. Bioinformatics for health care and diseases
2. Computational genomics/proteomics
3. Computational systems for modeling biological processes
4. Biomedical engineering
5. Biomedical image analysis
6. Biomedicine and e-health

This seventh edition of IWBBIO was organized by the Universidad de Granada. We wish to thank to our main sponsor and the institutions, the Faculty of Science, Department of Computer Architecture and Computer Technology, and CITIC-UGR from the University of Granada for their support and grants. We wish also to thank to the editors of different international journals for their interest in editing special issues from the best papers of IWBBIO.

We would also like to express our gratitude to the members of the various committees for their support, collaboration, and good work. We especially thank the Organizing Committee, Program Committee, the reviewers and special session organizers. We also want to express our gratitude to the EasyChair platform. Finally, we want to thank Springer, and especially Alfred Hofmann and Anna Kramer for their continuous support and cooperation.

May 2019

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