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Preface

We are proud to present the set of final accepted full papers for the third edition of the IWBBIO conference "International Work-Conference on Bioinformatics and Biomedical Engineering" held in Granada (Spain) during April 25–27, 2018.

The IWBBIO 2018 (International Work-Conference on Bioinformatics and Biomedical Engineering) conference 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 2018 were to create a friendly environment that could lead to the establishment or strengthening of scientific collaborations and exchanges among attendees, and therefore, IWBBIO 2018 solicited high-quality original research papers (including significant work-in-progress) on any aspect of bioinformatics, biomedicine, and biomedical engineering.

We especially encouraged contributions dealing with 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; modelling and simulation and their application in life science domain, biomedicine, and biomedical engineering. The list of topics in the successive call for papers also evolved, resulting in the following list for the present edition:

1. Computational proteomics. Analysis of protein–protein interactions. Protein structure modelling. 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) 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 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 modelling.
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 3.1, Program Committee members or additional reviewer), 88 papers were accepted for oral, poster, or virtual presentation, according to the recommendations of the reviewers and the authors' preferences, and to be included in the LNBI proceedings.

During IWBBIO 2018, several Special Sessions were held. Special Sessions are a very useful tool for complementing the regular program with new and emerging topics of particular interest for the participating community. Special Sessions that emphasize multidisciplinary and transversal aspects, as well as cutting-edge topics, were especially encouraged and welcomed, and in this edition of IWBBIO 2018 were the following:

– **SS1. Generation, Management, and Biological Insights from Big Data.**
As the sequencing technologies develop, reducing the costs and increasing the accuracy, research in biological sciences is transformed from hypothesis-driven to data-driven approaches. Big data encompasses a generation of data ranging from DNA sequence data for thousands of individuals to single-cell data for thousands of cell types from an individual. This has moved the bottle-neck of the data generation down-stream to use these data to gain new knowledge, finally with an aim to improve the quality of human life. The important down-stream challenges with big data include development of strategies for efficient storage of big data making them findable, accessible, interoperable, and reusable (FAIR), to make them usable for research. The next step is the development of new methods including software and Web tools to make sense of big data. The final important step is to demonstrate that big data can indeed lead to new knowledge. This session will cover the research topics in all three aspects of big data described here.

Organizer: ***Dr. Anagha Joshi,*** *Group leader in the Division of Developmental Biology at the Roslin Institute, University of Edinburgh, UK.*

Website:

https://www.ed.ac.uk/roslin/about/contact-us/staff/anagha-joshi

– **SS2. Challenges in Smart and Wearable Sensor Design for Mobile Health.**
The analysis of data streams captured with biomedical sensors can be performed as an embedded procedure within the sensor or sensor network or at a later stage in a

receiving system. Currently, several systems reduce the number of signals monitored via sensors (e.g., when using wearable devices) in order to save energy. In this case, the pre-processing task is embedded into the sensor or close to it. As a result, fewer data are transferred but pattern matching becomes more complex since cross-reference data are missing and computing power is limited. This session should present new and emerging approaches.

Organizers: ***Prof. Natividad Martínez Madrid****, Head of the Internet of Things Laboratory and Director of the AAL-Living Lab at Reutlingen University, Germany.*

Prof. Juan Antonio Ortega*, Director of the Centre of Computer Scientific in Andalusia (Spain)* www.cica.es *and head of the research group IDINFOR (TIC223), University of Seville, ETS Ingeniería Informática, Spain.*

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

Websites:
http://iotlab.reutlingen-university.de
http://madeirasic.us.es/idinfor/
http://uc-lab.in.htwg-konstanz.de

– **SS3. Challenges and Advances in Measurement and Self-Parametrization of Complex Biological Systems.**
Our understanding of biological systems requires progress in the measurement techniques, methods, and principles of acquisition. The development of IT and physical resolution offers novel advanced probes, devices, or interpretation as well as more questions and possibilities. Automation of processing and analysis is increasing thanks to artificial intelligence and machine deep learning. The proper bioinformatic parametrization for the analysis of complex systems continues toward automatic or self-setting of the acquired biophysical attributes.
This special section provided a discussion on novel techniques and measurement devices, emerging challenges for complex systems, open solutions, and future visions. The broad examples from self-parametric results supported the discussion with practical applications.

Organizer: ***Dipl-Ing. Jan Urban****, PhD, Head of Laboratory of Signal and Image Processing, University of South Bohemia in Ceské Budejovice, Faculty of Fisheries and Protection of Waters, South Bohemian Research Center of Aquaculture and Biodiversity of Hydrocenoses, Institute of Complex Systems, Czech Republic.*

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

– **SS4. High-Throughput Bioinformatic Tools for Medical Genomics.**
Genomics is concerned with the sequencing and analysis of an organism's genome taking advantage of the current, cost-effective, high-throughput sequencing

technologies. Their continuous improvement is creating a new demand for 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 invited 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, orthologues, genetic markers, controlled vocabulary (GO, KEGG, InterPro)
- Tools for biological enrichment in non-model organisms
- Tools for gene expression studies
- Tools for Chip-Seq data
- Tools for "big data" analyses
- Tools for integration in workflows

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.*

– **SS5. Drug Delivery System Design Aided by Mathematical Modelling and Experiments.**
A drug delivery system is designed to releases controlled amount of drugs to a specific target area. To devise optimization strategies for targeted drug delivery the combined action of various processes needs to be well understood. Mathematical modelling offers a valuable tool when evaluating potential drug-carrying materials coupled with rate-controlling coatings. When applied to experimental data, simulations can yield valuable insight and guide further research with the aim of identifying and evaluating key drug release mechanisms. Although diffusion is often a primary drug release process, other effects such as binding and dissolution as well as effects occurring at material interfaces are no less important in describing various rate-controlling release mechanisms.

Considered systems include: intraocular- and soft contact lenses, orthopedic implants, arterial stents, and transdermal patches.

Organizers: ***PhD candidate Kristinn Gudnason****, Faculty of Industrial Engineering, Mechanical Engineering and Computer Science, University of Iceland, Iceland.*

Prof. Fjola Jonsdottir*, Faculty of Industrial Engineering, Mechanical Engineering and Computer Science, University of Iceland, Iceland.*

Prof. Emeritus Sven Sigurdsson*, Faculty of Industrial Engineering, Mechanical Engineering and Computer Science, University of Iceland, Iceland.*

Prof. Mar Masson*, Faculty of Pharmaceutical Science, University of Iceland, Iceland.*

– **SS6. Molecular Studies on Inorganic Nanomaterials for Therapeutical and Diagnosis Applications.**
Nanostructured material science with natural origins is becoming a hot topic in nanomedicine for addressing toxicity and high cost limitations. The absorption of pharmaceutical drugs in natural inorganic nanostructured solids is very useful for controlled delivery of bioactive compounds. Molecular modelling and analytical spectroscopic techniques are well-established research fields for the characterization of these materials. This approach is becoming of great interest in the studies of these nanocomposites and the interactions of organics on the surfaces of the inorganic solids in health applications. The aim of this session is to gather professionals from a wide scope of scientific disciplines to better understand molecular aspects of nanocomposite components behavior and drug design. This interdisciplinary session included contributions from computational chemistry (empirical potentials, quantum, coarse-grained, etc.), NMR, infrared, and Raman spectroscopies, as well as X-ray-diffraction/neutron/synchrotron techniques.
This special session has a multidisciplinary nature and is not easy to be included in one of the congress topics owing to its transversal aim connected with several topics of the congress: computational proteomics (protein structure modelling), biomedicine (biomedical computing, nanomedicine), biomedical engineering (bio-nanotechnology), computational systems for modelling biological processes (simulation and visualization of biological systems), health care and diseases (drug design and computational immunology).
The aim of this special session is to show the potential application of computational modelling methods in nanomedicine for experimental researchers and, at the same time, for theoreticians diagnosing possible complementary tools for experiments, generating useful discussions between experimentalists and theoreticians to promote future scientific collaborations.

Organizers: ***Dr. C. Ignacio Sainz-Díaz****, Instituto Andaluz de Ciencias de la Tierra, CSIC/UGR, Granada, Spain.*

***Dr. Carola Aguzzi**, Departamento de Tecnología Farmacéutica, Universidad de Granada, Granada, Spain.*

– **SS7. Little-Big Data. Reducing the Complexity and Facing Uncertainty of Highly Underdetermined Phenotype Prediction Problems.**
Phenotype prediction problems have a very underdetermined character since the number of samples is always much lower in size than the number of genes/genetic probes/SNPs/etc., that are monitored to explain a given phenotype. This generates decision problems that have a huge uncertainty space. This includes a great variety of problems with great impact in translational medicine, such as the analysis of mechanism of action of genes in disease progression, the investigation of new therapeutic targets, the analysis of secondary effects, treatment optimization, as well as analysis of the effect of mutations in the transcriptome and in proteomics, etc.
The objective of the session was to present novel computational approaches to reduce the complexity of high-dimensional genetic data while keeping the main information content. Applications in cancer and genomics as well as rare and neurodegenerative diseases were welcome. In particular, the design of new methods to perform the robust analysis of pathways involved in disease development were one of the main topics addressed in this session.

Organizer: ***Prof. Juan Luis Fernández-Martínez**, Mathematics Department, Applied Mathematics Section, Director of the Group of Inverse Problems, Optimization and Machine Learning, University of Oviedo, Spain.*

– **SS8. Interpretable Models in Biomedicine and Bioinformatics.**
In a very short period of time, many areas of science have made a sharp transition toward data-driven methods. This new situation is clear in the life sciences and, as particular cases, in biomedicine, bioinformatics, and health care.
You could see this as a perfect scenario for the use of data analytics, from multivariate statistics to machine learning (ML) and computational intelligence (CI), but this scenario also poses some serious challenges. One of them takes the form of (lack of) interpretability/comprehensibility/explainability of the models obtained through data analysis. This could be a bottleneck especially for complex nonlinear models, often affected by what has come to be known as the "black box syndrome." In some areas such as medicine and health care, not addressing such challenges might seriously limit the chances of adoption, in real practice, of computer-based medical decision support systems (MDSS).
Interpretability and explainability have become hot research issues, and there are different reasons for this: One of them is the soaring success of deep learning artificial neural networks in recent years. These models risk not being adopted in areas where human decision is key and that decision must be explained as they are extreme "black box" cases. Another reason is the implementation of the European Union directive for General Data Protection Regulation (GDPR). Enforced in April 2018, it mandates a right to explanation of all decisions made by automated or artificially intelligent algorithmic systems. Needless to say, this directly involves data analytics and it is likely to have an impact on health care, medical

decision-making, and even in bioinformatics through the use of genomics in personalized medicine.
In this session, we called for papers that broach the topics of interpretability/comprehensibility/explainability of data models (with a non-reductive focus on ML and CI) in biomedicine, bioinformatics, and health care, from different viewpoints, including:

- Enhancement of the interpretability of existing data analysis techniques in problems related to biomedicine, bioinformatics, and health care
- New methods of model interpretation/explanation in problems related to biomedicine, bioinformatics, and health care
- Case studies biomedicine, bioinformatics, and health care in which interpretability/comprehensibility/explainability is a key aspect of the investigation
- Methods to enhance interpretability in safety-critical areas (such as, for instance, critical care)
- Issues of ethics and social responsibility (including governance, privacy, anonymization) in biomedicine, bioinformatics, and health care

Organizers: ***Prof. Alfredo Vellido,*** *Intelligent Data Science and Artificial Intelligence (IDEAI) Research Center, Universitat Politècnica de Catalunya, Barcelona, Spain.*

Prof. Sandra Ortega-Martorell, *Department of Applied Mathematics, Liverpool John Moores University, Liverpool, UK.*

Prof. Alessandra Tosi, *Mind Foundry Ltd., Oxford, UK.*

Prof. Iván Olier Caparroso, *MMU Machine Learning Research Lab, Manchester Metropolitan University, Manchester, UK.*

– **SS9. Medical Planning: Management System for Liquid Radioactive Waste in Hospital Design.**
In tertiary hospitals where nuclear medicine services have been introduced, the radioactive materials used in diagnosis and/or treatment need to be handled. The hospital design and medical planning should consider these materials and their policy for treatment. Nuclear waste has been divided into solid and liquid based on the materials used and on their half-life times, which start from a few minutes to years.
In our study, the most common radioactive liquid materials (waste) were treated by smart systems that detect the material and based on its HLT (activities) will be distributed in shielded storage tanks to the sewage treatment plant (STP) of the hospital after keeping them for the required times. The location and capacity of these tanks together with their monitoring and control system should be considered in the design stage that determines the treatment processes.

Motivation and objectives for the session: The nuclear medicine department should be considered in the design stage and its space program. The location and capacity of storage tanks and their drainage lines should be considered in hospital.

Organizer: ***Dr. Khaled El-Sayed****, Assistant Professor of Biomedical Engineering, Department of Electrical and Medical Engineering, Benha University, Egypt.*

– **SS10. Bioinformatics Tools to Integrate Omics Dataset and Address Biological Question.**
Methodological advances in 'omics' technologies allow for the high-throughput detection and monitoring of the abundance of several biological molecules. Several 'omics' platforms are being used in molecular biology and in clinical practice for the understanding of molecular mechanisms underlying specific disease as well as for identifying trustworthy diagnostic/prognostic markers.
Omics strategies include: genomics, which aims to characterize and quantify a set of genes within a single cell of an organism; transcriptomics, which analyzes the levels of mRNA transcripts; proteomics, which includes the identification of proteins and the monitoring of their abundance; metabolomics, which measures the abundance of small cellular metabolites; interactomics, and many others. Although more informative, no single 'omics' analysis may fully unveil the complexities of a specific biological question, therefore, to achieve a more comprehensive "picture" of biological processes, experimental data made on different layers have to be integrated and analyzed. This special session aimed to provide a description of bioinformatics strategies aimed at integrating omics datasets to address biological questions.

Organizer: ***Dr. Domenica Scumaci****, PhD Laboratory of Proteomics, Department of Experimental and Clinical Medicine, Magna Græcia University of Catanzaro, Italy.*

– **SS11. Understanding the Mechanisms of Variant Effects on Human Disease Phenotype.**
Modern sequencing technologies have enabled whole-genome sequencing and detailed quantification of germline and somatic variations, many of which are related to human disease. However, these data are necessary but not sufficient for understanding the cause and effect of these variations as well as their mechanisms of involvement in human diseases phenotypes. Disease-related variants can have an impact on DNA, RNA, and protein functions and may lead to impaired replication, transcription, signal transduction, and epigenetic regulation. This session exploited computational approaches related to inferring the effects of human mutations on proteins, biomolecular interactions, and cellular pathways with the goal of elucidating mechanistic aspects of disease causative variants.

Organizer: ***Anna Panchenko****, PhD Head, Computational Biophysics Group Computational Biology Branch, National Center for Biotechnology Information, National Institutes of Health, Bethesda, USA.*

Website:
https://www.ncbi.nlm.nih.gov/CBBResearch/Panchenko/

In this edition of IWBBIO, we were honored to have the following invited speakers:

1. Prof. Joaquin Dopazo, Fundacion Progreso y Salud, Clinical Bioinformatics Research Area, Seville, Spain
2. Prof. Luis Rueda, School of Computer Science, Pattern Recognition and Bioinformatics Lab, Windsor Cancer Research Group, University of Windsor
3. Dr. Anagha Joshi, Bioinformatics Group Leader, Developmental Biology Division, The Roslin Institute, University of Edinburgh, UK
4. Prof. FangXiang Wu, SMIEEE Professor, Division of Biomedical Engineering, Department of Mechanical Engineering, College of Engineering, University of Saskatchewan, Canada
5. Prof. Jiayin Wang, Xi'an Jiaotong University, China

It is important to note, that for the sake of consistency and readability of the book, the presented papers are classified under 17 chapters. The organization of the papers is in two volumes arranged following the topics list included in the call for papers. The first volume (LNBI 10813), entitled *Advances in Computational Intelligence. Part I* is divided into 11 main parts and includes the contributions on:

1. Bioinformatics for health care and diseases
2. Bioinformatics tools to integrate omics datasets and address biological questions
3. Challenges and advances in measurement and self-parametrization of complex biological systems
4. Computational genomics
5. Computational proteomics
6. Computational systems for modelling biological processes
7. Drug delivery system design aided by mathematical modelling and experiments
8. Generation, management, and biological insights from big data
9. High-throughput bioinformatic tools for medical genomics
10. Next-generation sequencing and sequence analysis
11. Interpretable models in biomedicine and bioinformatics

In the second volume (LNBI 10814), entitled *Advances in Computational Intelligence. Part II* is divided into six main parts and includes the contributions on:

1. Little-big data. Reducing the complexity and facing uncertainty of highly underdetermined phenotype prediction problems
2. Biomedical engineering
3. Biomedical image analysis
4. Biomedical signal analysis
5. Challenges in smart and wearable sensor design for mobile health
6. Health care and diseases

This sixth edition of IWBBIO was organized by the Universidad de Granada together with the Spanish Chapter of the IEEE Computational Intelligence Society. We

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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 local Organizing Committee, Program Committee, the reviewers, and special session organizers. We also want to express our gratitude for the EasyChair platform. Finally, we want to thank Springer, and especially Alfred Hoffman and Anna Kramer for their continuous support and cooperation.

April 2018

Ignacio Rojas
Francisco Ortuño

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