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Andrea Bracciali · Giulio Caravagna  
David Gilbert · Roberto Tagliaferri (Eds.)


# Computational Intelligence Methods for Bioinformatics and Biostatistics


13th International Meeting, CIBB 2016  
Stirling, UK, September 1–3, 2016  
Revised Selected Papers

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# Preface

The 13th annual edition of the international meeting on Computational Intelligence methods for Bioinformatics and Biostatistics (CIBB 2016) built upon the tradition of the CIBB conference series and provided a multi-disciplinary forum open to researchers interested in the application of computational intelligence, in a broad sense, to open problems in bioinformatics, biostatistics, systems and synthetic biology, medical informatics, as well as computational approaches to life sciences in general.

In line with the spirit of CIBB, the 2016 meeting brought together researchers from different communities who address problems from different, but connected and often overlapping, perspectives. CIBB 2016 tackled the difficult task of bridging different backgrounds by providing an inclusive venue to discuss advances and future perspectives in different areas. It also fostered interaction between theory and practice, addressing both the theories underpinning the methodologies used to model and analyze biological systems, the practical applications of such theories, and the supporting technologies. Accordingly, participants at CIBB 2016 came from mathematical, computational, and medical backgrounds and institutions, both from academia and the private sector, offering collaboration opportunities and novel results in the areas of computational life sciences.

CIBB 2016 also offered a view on emerging and strongly developing trends and future opportunities at the edge of mathematics, computer and life sciences, such as synthetic biology, statistical investigation of genomic data, and applications to the understanding of complex diseases, such as cancer, and therapy opportunities. Along these lines, six keynote speakers, prominent scholars in their fields, presented the latest advances of their research within the context of their area of interest, and provided insights into open problems and future directions of general interest for the field. While papers in the main conference track addressed a rich set of open problems at the forefront of current research, the conference hosted six further special sessions on specific themes: biomedical databases, synthetic cell biology, high-performance computing in genetics, modelling for systems biology and medicine, survival analysis, and statistical inference in biological models. Researchers from Europe, Asia, USA, and Africa attended the conference. CIBB 2016 was made possible by the efforts of the Organizing, Program, and Steering Committees and by the support of sponsors and participants. CIBB 2016 was held in Stirling, UK, during September 1–3, 2016 (<http://www.cs.stir.ac.uk/events/cibb2016/>). With the continued support of the community, the next edition of CIBB will be held in Cagliari, Italy.

Overall, 61 contributions were submitted for consideration to CIBB 2016, amongst which 49 were invited for an oral presentation at the conference, after a first round of reviews (at this stage, each paper received an average of 3.7 reviews from the Program Committee and about 30 additional referees). Following the conference, selected papers were invited for further submission, after feedback and discussion from the conference.

This volume collects the papers that were accepted after a further round of reviews (2.5 for each paper, on average).

From 2004 to 2007, CIBB had the format of a special session of larger conferences, namely, WIRN 2004 in Perugia, WILF 2005 in Crema, FLINS 2006 in Genoa, and WILF 2007 in Camogli. Given the great success of the special session at WILF 2007 that included 26 strongly rated papers, the Steering Committee decided to turn CIBB into an autonomous conference starting with the 2008 edition in Vietri. The following editions in Italian venues were held in Genoa (2009), Palermo (2010), and Gargnano (2011). Until 2012, CIBB meetings were held annually in Italy with an increasing number of participants. CIBB 2012 was the first edition organized outside Italy, in Houston, then in Nice, France (2013), Cambridge, UK (2014), and Naples, Italy (2015). A rigorous peer-review selection process is applied every time to ultimately select the papers included in the program of the conference, in the conference proceedings published in the LNBI-LNCS book series by Springer, and in some cases, selected papers were published in special issues of well-qualified international journals, such as *BMC Bioinformatics*.

June 2017

Andrea Bracciali  
Giulio Caravagna  
David Gilbert  
Roberto Tagliaferri

# Organization

CIBB 2016 was jointly organized by the Computing Science and Mathematics, University of Stirling, UK, and the Dipartimento di Informatica, University of Salerno, Italy.

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Antonietta Mira	IDIDS, Università della Svizzera italiana and Università dell'Insubria, Italy
Bud Mishra	Courant Institute of Mathematical Sciences, NYU School of Medicine, NYU Mt. Sinai School of Medicine, USA
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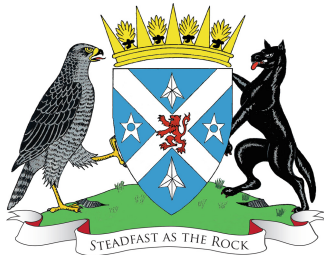
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This conference was organized with the support of EasyChair conference system.

# **Keynote Abstracts**

# Accelerating Synthetic Biology via Software and Hardware Advances

Natalio Krasnogor

School of Computing Science, Newcastle University

In this talk I will discuss recent work done in my lab that contributes towards accelerating the

specify → design → model → build → test & iterate

biological engineering cycle. This will describe advances in biological programming languages for specifying combinatorial DNA libraries, the utilisation of off-the-shelf microfluidic devices to build the DNA libraries as well as data analysis techniques to accelerate computational simulations.

**Professor Natalio Krasnogor** is Professor of Computing Science and Synthetic Biology, co-directs Interdisciplinary Computing and Complex Biosystems (ICOS) research group and is director of Newcastle's Centre for Synthetic Biology and the Bioeconomy (CSBB). Krasnogor holds an EPSRC Leadership Fellowship in Synthetic Biology (SB) (EP/J004111/1 - 1.1M), is the PI on the EPSRC programme grant "Synthetic Portabolomics" (EP/N031962/1 - 4.3M) and is the overall lead in the EPSRC Synthetic Biology ROADBLOCK (EP/I031642/1, EP/I031812/1, EP/I03157X/1 - 1.7M) project involving Newcastle, Nottingham, Sheffield, Warwick and Bradford Universities. With expertise in Synthetic Biology, complex systems and machine intelligence, he attracted 4.5M as PI from UKRC and EU. Krasnogor gave several keynote talks (e.g. IEEE CEC, PPSN, GECCO, etc); has 160+ publications (H-index 36), with many papers in the top 0.1% and 1% for number of citations in computing science and also papers in Nature Biotech, Nature Chemistry, PNAs, NAR, EMBO Journal, etc. He won several best papers prizes as well as Bronze, Silver and Gold awards of the American Computing Society's (ACM) HUMIES and ACM's Impact award. From 2012 to 2014 he was the Science Director of the European Centre for Living Technologies (Italy) and was distinguished visiting professor at Ben Gurion University (Israel) in 2009 and Weizmann Institute of Science (Israel) in 2010, 2012 and 2013. Krasnogor current interests in Synthetic Biology are in the development of artificial intelligence techniques, including data analytics, the design of programming languages for biological engineering and research at the interface of nano and bio technology.

# (Cancer) Genomics via (Sub)Optical Mapping

Bud Mishra

Computer Science, Mathematics, Engineering and Biology, Courant Institute,  
Tandon School of Engineering, and NYU School of Medicine

The dream of a powerful integrated computational framework, only hinted at in Ibn Sina's Canon, can now be fulfilled at a global scale as a result of many recent advances: foundational advances in statistical inference; hypothesis-driven experiment design and analysis and the dissemination of peer-reviewed publications among communities of scientists; distributed large-scale databases of scientific and auxiliary experimental data; algorithmic approaches to model building and model checking; machine learning approaches to generate large number of hypotheses, and multiple hypotheses testing to tame computational complexity and false-discovery rates, etc. We will focus on an application centered on cancer - "the emperor of all maladies."

The topics this talk will cover include:

- Probabilistic causation
- Causal analysis of Cancer genome data
- Kernel based methods for survival analysis
- Improved single-cell/single-molecule data via SubOptical Mapping
- CHA and Therapy design
- Immuno-therapy
- Liquid Biopsies

**Professor Bud Mishra** is an American-Indian technologist, educator and mentor. He is currently a professor of computer science and mathematics at NYU's Courant Institute of Mathematical Sciences, professor of engineering at NYU's Tandon School of Engineering, professor of human genetics at Mt. Sinai School of Medicine, visiting scholar at Cold Spring Harbor Laboratory and a professor of cell biology at NYU School of Medicine. Prof. Mishra has a degree in Science from Utkal University, in Electronics and Communication Engineering from IIT, Kharagpur, and MS and PhD degrees in Computer Science from Carnegie-Mellon University. He has advisory experience in Computer and Data Science (ATTAP, brainiad, Genesis Media, Pype-stream, and Tartan Laboratories), Finance (Instadat, PRF, LLC, and Tudor Investment), Robotics and Bio- and Nanotechnologies (Abraxis, Bioarrays, InSilico, MRTech, OpGen and Seqster). He has advised and mentored more than 35 graduate students and post-docs in the areas of computer science, robotics and control engineering, applied mathematics, finance, biology and medicine. He holds 21 issued and 23 pending patents in areas ranging over robotics, model checking, intrusion detection, cyber security, emergency response, disaster management, data analysis, biotechnology, nanotechnology, genome mapping and sequencing, mutation calling, cancer biology, fintech, adtech, internet architecture and linguistics. His pioneering work includes: first

application of model checking to hardware verification; first robotics technologies for grasping, reactive grippers and work holding; first single molecule genotype/haplotype mapping technology (Optical Mapping); first analysis of copy number variants with a segmentation algorithm, first whole-genome haplotype assembly technology (SUTTA), first clinical-genomic variant/base calling technology (TotalRecaller), and current work in progress continuing in the areas of liquid biopsies, cancer data, cyber security, cryptography, financial engineering and internet of the future. He is a fellow of IEEE, ACM and AAAS, a Distinguished Alumnus of IIT-Kgp, and a NYSTAR Distinguished Professor.

# Statistical Inference on Large-Scale Gene Duplication Networks

Antonietta Mira

IDIDS, Università della Svizzera italiana and Università dell'Insubria

Many systems of scientific interest can be investigated as networks, where network nodes correspond to the elements of the system and network edges to interactions between the elements. Increasing availability of large-scale biological data and steady improvements in computational capacity are continuing to fuel the growth of this field. Network models are now used commonly to investigate biological complexity at the systemic level. Gene duplication is one of the main drivers of the evolution of genomes, and network models based on gene duplication were one of the first large-scale models used in systems biology. An attractive feature of some of these so-called duplication-divergence models is their analytical tractability, but there is typically no statistically principled way to estimate their model parameters from empirical data. This is a reflection of a more general divide between the two prominent paradigms to the modeling of networks, which are the approach of mechanistic networks models and the approach of statistical network models. Mechanistic network models assume that the microscopic mechanisms governing network formation and evolution at the level of individual nodes are known, and questions often focus on understanding macroscopic features that emerge from repeated application of these known mechanisms. The statistical approach, in contrast, often starts from observed network structures and attempts to infer some aspects about the underlying data generating process. Mechanistic network models provide insight into how the network is formed and how it evolves at the level of individual nodes, but as mechanistic rules typically lead to complex network structures, it is difficult to assign a probability to any given network realizations that a mechanistic model may generate. Because of this difficulty, there is typically no closed form expression for likelihood for these models and, consequently, likelihood based inference for learning from data is not possible. We have developed a principled statistical framework, based on Approximate Bayesian Computation, to bring some of the mechanistic network models into the realm of statistical inference. This approach is feasible because given a set of parameter values, it is easy to sample network configurations from most mechanistic models. I will introduce this general framework and demonstrate its application to large-scale gene duplication networks, where it can be used to infer model parameters, and their associated uncertainties, for mechanistic network models from empirical data.

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Joint work with Jukka-Pekka Onnela, Department of Biostatistics, Harvard



**Antonietta Mira** is a professor of statistics, and co-founder and co-director of the InterDisciplinary Institute of Data Science, IDIDS, at Universit della Svizzera italiana, where she also served as the Vice-Dean in the Faculty of Economics (2013–2015). She is a fellow of the International Society for Bayesian Analysis, a member of the Istituto Lombardo Accademia di Scienze e Lettere, a visiting fellow of the Isaac Newton Institute for Mathematical Sciences at Cambridge University (2014 and 2016), and of the Queensland University of Technology (2016–2019). She is the principal investigator on several projects at the Swiss National Science Foundation and a member of multiple scientific committees representing her areas of expertise: Bayesian statistical models and efficient Monte Carlo simulation algorithms and theory. She has been member of the board of the ISBA Section on Bayesian Computation since 2013 and has been member of the scientific program committee and of the organizing committee of the joint international meeting of the Institute of Mathematical Statistics/International Society for Bayesian Analysis, aka MCMSki. Her current research focuses on data science and methodological and computational statistics, both of which have a clear interdisciplinary scope across social science, biology, genetics, economics and finance. She is often invited to talk at international scientific conferences. She served on the editorial board of Bayesian Analysis, Statistica Sinica and the Journal of Computational and Graphical Statistics as has been Chief Guest Editor for two special issues of Statistics and Computing. She has been involved in public engagement (such as EXPO Milano 2015), has delivered public lectures on several science festivals, and is the scientific lead for the exhibit Numbed by Numbers! Antonietta holds a PhD in Computational Statistics (1998, University of Minnesota, US) and a Doctorate in Methodological Statistics (1995, University of Trento, Italy). She has earned her Bachelor's in Economics, *summa cum laude*, from the University of Pavia, Italy. Her work has been published in over 60 scientific articles and she is co-author of the book *Mathematical-Magic* (Aboca, 2012).

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