

Combinatorial optimisation models for analysing biological data sets

A/Prof Regina Berretta
Deputy Head of School of Electrical Engineering and Computer Science,
Priority Research Centre for Bioinformatics, Biomarker Discovery and
Information Based Medicine
Information Based Medicine Program, Hunter Medical Research Institute

The University of Newcastle, Australia

Abstract: This talk will present combinatorial optimisation models and algorithmic techniques that have been developed to analyse large datasets.

First, the presentation will focus on an approach, based on a combinatorial optimisation problem (called the (α, β) -k-Feature Set Problem) to deal with the problem of selecting groups of features, such as genes, that discriminate between different existing classes. We will illustrate the application of these models using different variations of the model in several datasets.

Next, the presentation will illustrate how a classical and well-known combinatorial optimisation problem; the Quadratic Assignment Problem (QAP), is employed as a mathematical model to produce a visualization of a data set, based on the relationships between the elements in the data set. The visualization method can also incorporate the results of a clustering algorithm to facilitate the process of data analysis.

Bio: A/Prof Regina Berretta is Deputy Head of School of Electrical Engineering and Computer Science and one of the founding academics of the Priority Research Centre for Bioinformatics, Biomarker Discovery and Information Based Medicine, The University of Newcastle, Australia. She is also a member of the Information Based Medicine Program at Hunter Medical Research Institute. A/Prof Berretta holds degrees in Computational and Applied Mathematics, a Master and PhD in the area of metaheuristic methods for solving combinatorial optimisation problems arisen in production planning at University of Campinas, Brazil. Her main research interest is in the development of mathematical models and computational methods to analyse biological data. She has a substantial expertise in the development of heuristics and metaheuristics for tackle complex combinatorial optimisation problems in several areas (production planning, education timetable, functional genomics, etc). She has published more than 60 papers and was awarded more than 20 competitive grants.

Personalized Information-based Medicine: Huge challenges, massive opportunities and some lessons learned

Prof Pablo Moscato
School of Electrical Engineering and Computer Science,
Priority Research Centre for Bioinformatics, Biomarker Discovery and
Information Based Medicine
Information Based Medicine Program, Hunter Medical Research Institute
The University of Newcastle, Australia

Abstract: A recent report from the McKinsey Global Institute highlights the top six disruptive technologies with highest economic impact: mobile internet, automation of knowledge work, Internet of Things, Cloud, Advanced robotics and Autonomous and near-autonomous vehicles. A close seventh is at the core of information-based medicine, next-generation genomics. These seven technologies account for an estimated value which is at least 28 trillion US dollar a year.

All of them share with Information-based Medicine the need of analyzing large datasets, with "Big Data" being the current buzzword. As such, the need of querying a large variety of digital data and the use of artificial-intelligence and optimization software to find novel insights is not considered a separate technology, but a omnipresent requirement across all technologies.

Personalized Medicine aims at putting the best interests of the patient/individual, at the centre of all medical decisions, institutional practices, and/or drugs and treatments that necessarily be "tailored" to the individual profile. Clearly next-generation genomics is pertinent here, but the automation of knowledge work will also prove vital.

These two perspectives for the future of Medicine should contribute to each other. The novel technologies generate an ocean of data, but without strategic approaches for knowledge reuse they do not deliver for the promise. The huge perceived challenges generally involve large optimization. However, the implicit challenge is the development of new mathematical models that contemporize the needs of personalized medicine, who aims at the best diagnostic and treatment, and Information-based Medicine, with the needs of institutions/governments that aim at delivering the best health policies while minimizing global intervention costs operating under budget constraints.

Bio: Australian Research Council Future Fellow Prof. [Pablo Moscato](#) is the founding co-director of the Priority Research Centre for Bioinformatics, Biomarker Discovery and Information-based Medicine (2006-) and the funding director of Newcastle Bioinformatics Initiative (2002-2006) of The University of Newcastle. He is also Chief Investigator of the Australian Research Council Centre in Bioinformatics.

Prof. Moscato has been working in Evolutionary Computation for 25 years, and in heuristic methods for Operations Research problems since 1985. His work and ideas have been highly influential in a large number of scientific and technological fields and his manuscripts have been cited more than 4,211 times (data from Google Scholar). The journal "Memetic Computing" is largely dedicated to a methodology he championed since early work with Mike Norman at Caltech in 1988 (memetic algorithms). He is one of Australia's most cited computer scientists.

In the past seven years he has introduced a unifying hallmark of cancer progression based on the changes of information theory quantifiers, developed a novel mathematical model and an associated solution procedure based on combinatorial optimization techniques to identify drug combinations for cancer therapeutics. He has also identified proteomic signatures to predict years in advance the clinical symptoms of Alzheimer's Disease among other 'firsts'. His current fellowship supports him for four years (2012-2016) to develop memetic algorithms for multiobjective optimization problems in clinical bioinformatics for personalized and translational medicine.