Guest Editorial

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# Computational Intelligence Techniques in Bioinformatics and Bioengineering

The field around Bioinformatics and Bioengineering is rich and includes important and diverse problems, such as protein structure prediction, systems and synthetic biology, feature discovery and induction, healthcare informatics, biomarker discovery, and development of personalized medicine and treatment, amongst others. Many of the above problems can be framed as optimization, modeling and/or learning problems that are too difficult to tackle via classical techniques. Consequently, a consensus is emerging that current state-of-the-art approaches, such as sampling-based schemes in the Rosetta suite for macromolecular modeling, or classical mathematical programming methods, have reached a saturation point and are not very effective for vast multi-modal landscapes encountered in this domain.

**Many Bioinformatics and Bioengineering problems can be framed as optimization, modeling and/or learning problems that are too difficult to tackle via classical techniques.**

Over the past decade, it has become clear that increases in computational power alone will not be sufficient to combat this problem, and that there is a need for the development of specialized search and learning procedures that exploit problem-specific features and are capable of reusing information gathered during the problem solving procedure.

The field around optimization and learning via computational intelligence offers a repertoire of candidate techniques for global optimization and learning, as well as a rich body of theoretical and empirical work relating to their tuning and performance in different problem domains. Large parts of this expertise are yet to make their debut in the domain of bioinformatics and bioengineering, as the knowledge exchange between the two fields has been limited. It is only very recently that this boundary has started to break down, and promising preliminary applications have underlined the potential of this research direction. Given this, a special issue in a popular journal, such as IEEE Computational Intelligence Magazine, is particularly timely and will help further draw attention to this emerging research area.

The computational intelligence community in bioinformatics and bioengineering is fragmented and large. The aim of the special issue is to capture some of the ongoing interdisciplinary research that draws upon joint expertise in the domains of optimization and learning via computational intelligence techniques and bioinformatics and bioengineering. After a rigorous review process, two papers were selected for publication in the special issue.

The first paper, "*Identifying DNA methylation modules associated with a cancer by probabilistic evolutionary learning*" by Je-Keun Rhee, Soo-Jin Kim, and Byoung-Tak Zhang, aims at improving our understanding on the effects of DNA methylation on complex diseases. In particular, the paper focuses on identifying multiple interactions of many DNA methylation sites in the context of cancer. The authors demonstrate that computational intelligence (more precisely, an estimation of distribution algorithm-based evolutionary algorithm) can be used to identify high-order interactions of DNA methylated sites that are potentially relevant to a disease. The methodology has been validated successfully on array- and sequencing-based high-throughput DNA methylation profiling datasets.

The second paper, "*Augmentation of physician assessments with multi-omics enhances predictability of drug response: A case study of major depressive disorder*" by Arjun Athreya, Ravishankar Iyer, Drew Neavin, Liewei Wang, Richard Weinshilboum, Rima Kaddurah-Daouk, John Rush, Mark Frye, William Bobo, proposes a learning-augmented clinical assessment workflow to sequentially augment a physician's assessment of patients symptoms and their socio-demographic measures with heterogeneous biological measures to accurately predict treatment outcomes using machine learning and computational

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intelligence. Using real data from a clinical trial as a case study, the paper demonstrates that the proposed approach can yield significant improvements in the prediction accuracy for antidepressant treatment outcomes in patients with major depressive disorder, compared to using only a physician's assessment as the predictor. In other words, the paper argues that a properly tuned prediction model can be used to assess the therapeutic efficacy for a new patient prior to treatment. Ultimately, the approach proposed may find applications beyond psychiatry, for example, for predicting treatment outcomes for other medical conditions, such as migraine headaches or rheumatoid arthritis.

**There is a need for the development of specialized search and learning procedures that exploit problem-specific features and are capable of reusing information gathered during the search.**

We would like to use this opportunity to thank all the authors for submitting their high quality papers to the special issue, and all the reviewers for their invaluable contribution in assessing the submissions. Our final thanks go to the Editor-in-Chief of IEEE CIM, Hisao Ishibuchi, for the opportunity to publish the special issue and his support and advice throughout the process.

## Publication Spotlight

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"Reinforcement learning (RL) problems are hard to solve in a robotics context as classical algorithms rely on discrete representations of actions and states, but in robotics both are continuous. A discrete set of actions and states can be defined, but it requires an expertise that may not be available, in particular in open environments. It is proposed to define a process to make a robot build its own representation for an RL algorithm. The principle is to first use a direct policy search in the sensori-motor space, i.e., with no predefined discrete sets of states nor actions, and then extract from the corresponding learning traces discrete actions and identify the relevant dimensions of the state to estimate the value function. Once this is done, the robot can apply RL: 1) to be more robust to new domains and, if required and 2) to learn faster than a direct policy search. This approach allows to take the best of both worlds: first learning in a continuous space to avoid the need of a specific representation, but at a price of a long learning process and a poor generalization, and then learning with an adapted representation to be faster and more robust."

### IEEE Transactions on Emerging Topics in Computational Intelligence

*Insights on Transfer Optimization: Because Experience is the Best Teacher*, by A. Gupta, Y. S. Ong, and L. Feng, *IEEE Transactions on Emerging Topics in Computational Intelligence*, Vol. 2, No. 1, February 2018, pp. 51–64.

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"Traditional optimization solvers tend to start the search from scratch by assuming zero prior knowledge about the task at hand. Generally speaking, the capabilities of solvers do not automatically grow with experience. In contrast, however, humans routinely make use of a pool of knowledge drawn from past experiences whenever faced with a new task. This is often an effective approach in practice as real-world problems seldom exist in isolation. Similarly, practically useful artificial systems are expected to face a large number of problems in their lifetime, many of which will either be repetitive or share domain-specific similarities. This view naturally motivates advanced optimizers that mimic human cognitive capabilities; leveraging on what has been seen before to accelerate the search toward optimal solutions of never before seen tasks. With this in mind, this paper sheds light on recent research advances in the field of global black-box optimization that champion the theme of automatic knowledge transfer across problems. We introduce a general formalization of transfer optimization, based on which the conceptual realizations of the paradigm are classified into three distinct categories, namely sequential transfer, multitasking, and multiform optimization. In addition, we carry out a survey of different methodological perspectives spanning Bayesian optimization and nature-inspired computational intelligence procedures for efficient encoding and transfer of knowledge building blocks. Finally, real-world applications of the techniques are identified, demonstrating the future impact of optimization engines that evolve as better problem-solvers over time by learning from the past and from one another."