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Nature Inspired Cooperative Strategies for Optimization (NICSO 2013)

Springer

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Preface

The ability of computer scientist, engineers and practitioners to find sources of inspiration in nature to abstract metaphors suitable for problem solving has proven limitless. For instance, the rationale behind computational platforms such as cloud computing, whereby users access distributed computing power to exploit data sharing and information processing, has been observed in the lysogenic cycle which is one of the ways virus operate within cell DNA machinery to reproduce itself. Besides the already well-known applications on classification, learning and robotics to name but a few, nature inspired strategies became increasingly important to address challenges ranging at all scales from molecular reactions to social networks. As examples, we might mention that evolutionary algorithms already represent indispensable tools for the design optimisation of biochemical signalling pathways in synthetic biology and that cooperative spatio-temporal architectures are suitable approximations for modelling complex emergent behaviour seen in micro-scaled biological systems.

This book is a collection of research works presented in the VI International Workshop on Nature Inspired Cooperative Strategies for Optimization (NICSO) held in Canterbury, UK. Previous editions of NICSO were held in Granada, Spain (2006 & 2010), Acireale, Italy (2007), Tenerife, Spain (2008), and Cluj-Napoca, Romania (2011). The aim of NICSO 2013 is to provide a place where state-of-the-art research, latest ideas and emerging areas of nature inspired cooperative strategies for problem solving are vigorously discussed and exchanged among the scientific community. The contributions of this volume have undergone a strictly peer reviewed process by members of the international Programme Committee. The breadth and variety of articles report on nature inspired methods and applications such as Swarm Intelligence, Hyper-heuristics, Evolutionary Algorithms, Cellular Automata, Artificial Bee Colony, Dynamic Optimisation, Support Vector Machines, Multi-Agent Systems, Ant Clustering, Evolutionary Design Optimisation, Game Theory and other several Cooperation Models. In this edition, NICSO had three plenary lectures delivered by Dr. Alex A. Freitas, *Automating the Design of Data Mining Algorithms with Genetic Programming*, Dr. Angel Goñi Moreno, *Bacterial micromachines – Living logic circuits for computing*, and Dr. Leonardo Vanneschi, *Applications of Genetic Programming to Drug Discovery and Pharmacokinetics*.

Of course, neither NICSO 2013 or this book would exist without the help of many people and institutions. We wish to thank the authors for contributing with valuable articles to publication and each of the Programme Committee members for their dedicated time, suggestions and advice. In addition, we thank the financial support received from the Spanish Ministry of Economy and Competitiveness (project TIN2011-27696-C02-01), the Andalusian Government (project P11-TIC-8001), the European Regional Development Fund (ERDF), the School of Computing, University of Kent, and The European Commission FP7 Future

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Plenary Lectures

Dr. Alex A. Freitas

University of Kent, United Kingdom

Automating the Design of Data Mining Algorithms with Genetic Programming

Rule induction and decision-tree induction algorithms are among the most popular types of classification algorithms in the field of data mining. Research on these two types of algorithms produced many new algorithms in the last 30 years. However, all the rule induction and decision-tree induction algorithms created over that period have in common the fact that they have been manually designed, typically by incrementally modifying a few basic rule induction or decision-tree induction algorithms. Having these basic algorithms and their components in mind, we describe the use of Genetic Programming (GP), a type of evolutionary algorithm that automatically creates computer programs, to automate the process of designing rule induction and decision-tree induction algorithms. The basic motivation is to automatically create complete rule induction and decision-tree induction algorithms in a data-driven way, trying to avoid the human biases and preconceptions incorporated in manually-designed algorithms. Two proposed GP methods (one for evolving rule induction algorithms, the other for evolving decision-tree induction algorithms) are evaluated on a number of datasets, and the results show that the machine-designed rule induction and decision-tree induction algorithms are competitive with well-known human-designed algorithms of the same type.

Dr. Angel Goñi Moreno

National Center for Biotechnology, Spain

Bacterial micromachines – Living logic circuits for computing

Engineering Boolean logic circuits in bacteria is a major research theme of synthetic biology. By using living technology as DNA blocks or molecular wires we can mimic the behaviour of electronic devices. Examples of this engineering, such as logic gates, clock signals, switches, multiplexers or half adders have been successfully built inside bacteria. Just as the pioneers of computer technology quickly incorporated the early transistor into larger circuits, researchers in synthetic biology merge this genetic devices to achieve distributed computations within a microbial consortia. The rapid development of bacterial-based devices is accompanied by a need for computational simulations and mathematical modelling to facilitate the characterisation and design of such systems. Therefore,

computer sciences are mixed with synthetic biology (i.e. computational biology and bioinformatics) for two closely related purposes: 1) the design of devices, where the knowledge acquired in electronics since the beginning of computation is crucial; and 2) the desire to better understand the underlying biological substrate, giving answers to questions impossible to solve in a wet-lab. Up to now, bacterial micromachines are only in the form of basic computing devices. However, this machines are alive. Where is this engineering going?

Dr. Leonardo Vanneschi

ISEGI, Universidade Nova de Lisboa, Portugal

Applications of Genetic Programming in Drug Discovery and Pharmacokinetics

The success of a drug treatment is strongly correlated with the ability of a molecule to reach its target in the patients organism without inducing toxic effects. Moreover the reduction of cost and time associated with drug discovery and development is becoming a crucial requirement for pharmaceutical industry. Therefore computational methods allowing reliable predictions of newly synthesized compounds properties are of outmost relevance. In this talk, I discuss the role of Genetic Programming (GP) in predictive pharmacokinetics, considering the estimation of adsorption, distribution, metabolism, excretion and toxicity processes (ADMET) that a drug undergoes into the patients organism. In particular, I discuss the ability of GP to predict oral bioavailability (%F), median oral lethal dose (LD50) and plasma-protein binding levels (%PPB). Since these parameters respectively characterize the percentage of initial drug dose that effectively reaches the systemic blood circulation, the harmful effects and the distribution into the organism of a drug, they are essential for the selection of potentially effective molecules. In the last part of the talk, I show and discuss how recently defined geometric semantic genetic operators can dramatically affect the performances of GP for this kind of application, in particular on out-of-sample test data.

Table of Contents