Editorial

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D. Frank Hsu is the Clavius Distinguished Professor of Science at Fordham University in New York. He is the Vice Chair of the New York Chapter of the IEEE Computational Intelligence Society. His research interest in computing and informatics focuses on information fusion method and applications to information retrieval, target tracking, virtual screening and drug design, and protein structure prediction. He is a Fellow of the New York Academy of Sciences (NYAS) and the International Society of Intelligent Biological Medicine (ISIBM), and a Foundation Fellow of the Institute of Combinatorics and Applications (ICA).

Hui-Huang Hsu is an Associate Professor in the Department of Computer Science and Information Engineering at Tamkang University, Taipei, Taiwan. He received both his PhD and MS from the Department of Electrical and Computer Engineering at the University of Florida, USA, in 1994 and 1991, respectively. His current research interests are in the areas of machine learning, data mining, bio-medical informatics, ubiquitous intelligence and multimedia processing. He also edited a book titled "Advanced Data Mining Technologies

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Advances of Computing and Information Science technologies have facilitated, accelerated and promoted the research on molecular biology and medicine in the past few decades. To discover new knowledge in biomedical areas and to improve the quality of healthcare and medicine, the techniques and applications of artificial intelligence, machine learning, data mining and high-performance computing are extremely useful. This special issue aims to address and attract state-of-the-art solutions and novel attempts in the area of computational intelligence in biomedical informatics. The Guest Editors would like to thank all those who submitted papers to this special issue – *Computational Intelligence in Biomedical Informatics* for consideration. Also, we thank all the peer reviewers for their time and wonderful job, which has definitely helped to improve the quality and readability of this issue.

The first paper of this issue is 'Restructuring the Gene Ontology to emphasise regulative pathways and to improve gene similarity queries' by Alessia Visconti, Roberto Esposito and Francesca Cordero, Università di Torino, Italia. In this paper, authors introduce a technique for reorganising the database Gene Ontology. The reorganisation takes place in twofold: they arrange the regulative information into an abstract representation and they create edges that cross the sub-ontology boundaries. In addition, they show how an earlier work of the gene functional similarity can be adapted to work with the restructured Gene Ontology. Finally, they describe how their proposal fares when tested over several *Saccharomyces cerevisiae* pathways.

The second paper of this issue is 'Text mining and visualisation of Protein-Protein Interactions' by Flora S. Tsai, Nanyang Technological University, Singapore. In this paper, she provides an effective study of Protein-Protein Interactions (PPIs) to view and simulate protein interactions in three dimensions. This paper presents a text mining and visualisation framework for finding details of PPIs that occur within a particular subcellular location. By obtaining the sequence of the amino acids at the interface of a protein interaction, one can obtain a deeper understanding about the function of the protein.

The third paper of this issue is 'A hybrid metaheuristic for Closest String Problem', by Sayyed Rasoul Mousavi, Isfahan University of Technology, Iran. The Closest String Problem (CSP) is a combinatorial optimisation problem, which is to obtain a string whose hamming distance from the members of a given set of strings of the same length is minimal. It has applications, among others, in Bioinformatics, especially in drug target design. The problem is NP-hard and no exact polynomial-time algorithm is known for it. Consequently, approximation and (meta) heuristic algorithms have been proposed, which aim at achieving 'good', but not necessarily optimal, solutions. In this paper, a new metaheuristic algorithm is investigated for the problem, which is a hybridisation of constructive beam search and local search. The proposed algorithm is compared with three most recently published algorithms for the problem, outperforming them in more than 98% of the cases.

The fourth paper of this issue is 'Identification and classification of cocci bacterial cells in digital microscopic images' by P.S. Hiremath and Parashuram Bannigidad, Gulbarga University, India. In this paper, the objective of this study is to develop an automatic tool to identify and classify the different types of cocci bacterial cells in digital microscopic cell images. Geometric features are used to identify the arrangement of cocci bacterial cells, namely cocci, diplococci, streptococci, tetrad, sarcinae and staphylococci using 3-σ and K-NN classifiers. The current methods rely on the subjective reading of profiles by a human expert based on the various manual staining methods. In this paper, the authors propose a method for cocci bacterial cell classification by segmenting digital bacterial cell images and extracting geometric and statistical features for cell classification. The experimental results are compared with the manual results obtained by the microbiology expert and demonstrate the efficacy of the proposed method. The experimentation is done using SEM digital images of various cocci bacterial communities.

The fifth paper of this issue is 'LigSeeSVM: Ligand-based virtual Screening using Support Vector Machines and data fusion' by Yen-Fu Chen, Kai-Cheng Hsu, Po-Tsun Lin, D. Frank Hsu, Bruce S. Kristal and Jinn-Moon Yang, National Chiao Tung University, Taiwan, Fordham University, NY, USA and Harvard Medical School, MA, USA. Structure-based virtual screening of molecular compound libraries is a potentially powerful and inexpensive method for the discovery of novel lead compounds for drug development. That said, virtual screening is heavily dependent on detailed understanding of the tertiary or quaternary structure of the protein target of interest, including knowledge of the relevant binding pocket. Such information is often difficult or impossible to obtain. In contrast, ligand-based in silico drug screening can perform screening on drug targets whose three-dimensional structure is not yet determined. In their earlier work, authors demonstrated that the use of data fusion techniques strengthen virtual screening. Building on this data, they describe LigSeeSVM, a ligand-based screening tool using data fusion and support vector machines and termed. They combine Atom Pair (AP) structure descriptors and physicochemical (PC) descriptors to characterise compounds' features. They used SVM to generate SVM-AP model based on 825 AP descriptors and SVM-PC model based on 19 physicochemical descriptors. In this paper, authors combine SVM-AP and SVM-PC using rank-based information fusion to create LigSeeSVM model. LigSeeSVM was evaluated on five data sets including Thymindine Kinase (TK) substrates, Oestrogen Receptor (OR) antagonists, Oestrogen Receptor Agonists (ORA), GPCR and GABAA ligands. Their results suggest that LigSeeSVM is useful for ligand-based virtual screening and offers competitive performance to other ligand-based screening approaches.

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