Guest Editorial for Special Section on the 12th International Conference on Intelligent Computing (ICIC)

De-Shuang Huang, Vitoantonio Bevilacqua, and M. Michael Gromiha

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THIS special section includes a sub-selection of eight papers presented at the 12th International Conference on Intelligent Computing (ICIC) held at Lanzhou, China, during August 2-5, 2016. ICIC was formed to provide an annual forum dedicated to the emerging and challenging topics in artificial intelligence, machine learning, bioinformatics, and computational biology, etc. It aims to bring together researchers and practitioners from both academia and industry to share ideas, problems, and solutions related to the multifaceted aspects of intelligent computing.

This year, the conference received 639 submissions from 22 countries and regions. All papers went through a rigorous peer review procedure and each paper received at least three review reports. Based on the review reports, the Program Committee finally selected 236 research papers for presentation at ICIC 2016. Based on the novelty of the manuscripts, presentations, and originality, the authors of eight high quality papers were invited to submit an extended version and are included in this special section.

This special section is broadly classified into three categories, (i) structural analysis of protein complexes, (ii) prediction of residue-residue contacts, post translational modification sites, binding sites, and hotspot residues, and (iii) applications to specific diseases.

The opening article "Identification and Analysis of Key Residues in Protein–RNA Complexes" by A. Kulandaisamy, Ambuj Srivastava, Pradeep Kumar, R. Nagarajan, S. Binny Priya, and M. Michael Gromiha identified the key residues in protein-RNA complexes, which are involved in both stability and binding. They showed that key residues are enriched with the combination of polar, charged, aliphatic, and aromatic residues. Specifically, residues with similar chemical behavior have different preferences to be key residues, such that Arg, Tyr, Val, and Thr are preferred over Lys, Trp, Ile, and Ser, respectively.

Subsequently, focusing on prediction aspects, Hongjie Wu, Chengyuan Cao, Xiaoyan Xia, and Qiang Lü proposed a deep learning method for predicting residue-residue contacts in a protein in "Unified Deep Learning Architecture for Modeling Biology Sequence." They utilized bidirectional recurrent neural networks based on long short-term memory or a gated recurrent unit to capture long-range interactions. In addition, merging and pooling operators were used to identify short-range interactions.

Wenzheng Bao, Chang-An Yuan, Youhua Zhang, Kyungsook Han, Asoke K. Nandi, Barry Honig, and De-Shuang Huang utilized a combination of physical, chemical, statistical, and biological properties of a protein and proposed a novel framework for predicting the post translational modification sites in a protein in their paper "Mutli-Features Prediction of Protein Translational Modification Sites." They used the feature selection method for preprocessing the data and trained the featuers using multi-layered neural network and support vector machine to predict the potential post translational modified sites.

In "Sequence-Based Prediction of Putative Transcription Factor Binding Sites in DNA Sequences of Any Length," Wook Lee, Byungkyu Park, and Kyungsook Han proposed a computational method for predicting transcription factor binding sites in DNA using sequence based features such as composition, transition, and distribution of nucleotides and amino acids in DNA and protein sequences, respectively. They showed that the method is capable of predicting the transcription factor binding sites at high accuracy and will be useful for designing experiments.

In "Prediction of Hot Regions in PPIs Based on Improved Local Community Structure Detecting," Xiaoli Lin and Xiaolong Zhang devised a method for predicting hot regions in protein-protein interactions based on diverse biological properties. They followed different steps such as evaluation of features, creation of cassification model as well as detection and analysis of the conformation of hot regions in the prediction method. This algorithm is able to treat the missing residue nodes, control the local community boundaries to identify the hot regions reliably.

On the application side, Su-Ping Deng, Wenxing Hu, Vince D. Calhoun, and Yu-Ping Wang, developed a network-fusion based framework model using genomic,

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epigenomic, and neuroimaging data for identifying genetic biomarkers of complex diseases in their paper "Integrating Imaging Genomic Data in the Quest for Biomarkers of Schizophrenia Disease." Networks have been constructed for healthy and disease cases and genes with significant changes were determined as schizophrenia biomarkers by comparing their minimum spanning trees. This approach provides a general framework for discovering gene biomarkers of complex diseases, which could be used for diagnosis.

In "Continuous Petri Nets and microRNA Analysis in Melanoma," Giulia Russo, Marzio Pennisi, Roberta Boscarino, and Francesco Pappalardo developed a continuous Petri Net model for understanding the signalling cascades involved in melanoma development, such as MAPK and PI3K/AKT. They showed that hsa-mir-132 downregulates expression levels of p120RasGAP at high concentrations and it is significantly associated with clinical outcome in melanoma cancer genomic data sets of BRAF-mutated patients. The results suggest that targeting miRNAs through antisense oligonucleotides technology may enhance the action of BRAF inhibitors.

Jian Liu, Yuhu Cheng, Xuesong Wang, Xiaoluo Cui, Yi Kong, and Junping Du proposed a Low Rank Subspace Clustering model via Discrete Constraint and Hypergraph Regularization (DHLRS) for identifying cancer class in "Low Rank Subspace Clustering via Discrete Constraint and Hypergraph Regularization for Tumor Molecular Pattern Discovery." They adapted various steps and the procedure includes (i) learning the cluster indicators, (ii) approximating the low rank constraints, (iii) infering the complex relationship between genes and intrinsic geometrical structure of gene expression data in each subspace, and (iv) identifying the molecular pattern of tumor gene expression data sets. The results showed a good agreement with experiments on both synthetic data and real tumor gene expression data sets.

We would like to express our sincere thanks to the ICIC 2016 Program Committee members for their invaluable effort in making it a successful event. We would like to thank the external reviewers for volunteering their time to review the submissions to the conference and the special section. We would like to thank Aidong Zhang, the current editor-in-chief of the *IEEE/ACM Transactions on ComputationalBiology and Bioinformatics* (*TCBB*), for offering this opportunity for wider dissemination of the research presentedat ICIC 2016 in *TCBB*. Last, but not least, we would like to thank the authors of these eight articles for their time and effort in submitting their high quality work to ICIC and *TCBB*.

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De-Shuang Huang,
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Guest Editors

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De-Shuang Huang received the BSc degree from the Institute of Electronic Engineering, Hefei, China, in 1986, the MSc degree from the National Defense University of Science and Technology, Changsha, China, in 1989, and the PhD degree from Xidian University, Xian, China, in 1993, all in electronic engineering. During the 1993-1997 period, he was a postdoctoral student in the Beijing Institute of Technology and in the National Key Laboratory of Pattern Recognition, the Chinese Academy of Sciences, Beijing, China, respectively. In September, 2000, he joined the Institute of Intelligent Machines, the Chinese Academy of Sciences as the recipient of the "Hundred Talents Program of CAS". In September 2011, he entered into Tongji University as a chaired professor. From September 2000 to March 2001, he worked as a research associate with Hong Kong Polytechnic University. From August to September 2003, he visited George Washington University, Washington DC, USA, as a visiting professor. From July to December 2004, he worked as a university fellow with Hong Kong Baptist University. From March 2005 to March 2006, he worked as a research fellow in the Chinese University of Hong Kong. From March to July 2006, he worked as a visiting professor with the Queen's University of Belfast, UK. In 2007, 2008, and 2009, he worked as a visiting professor with Inha University, Korea, respectively. Currently, he is the visiting professor of the Liverpool John-Moore University, UK. In addition, he is the director of the Institute of Machines Learning and Systems Biology, Tongji University. He is currently a fellow of the International Association of Pattern Recognition (IAPR fellow), and a senior member of the IEEE and the International Neural Network Society (INNS). He was the 2015 International Joint Conference on Neural Networks (IJCNN 2015) general chair, July 12-17, 2015, Killarney, Ireland. He has published more than 190 journal papers. His current research interest includes bioinformatics, pattern recognition, and image processing.

Vitoantonio Bevilacqua received the bachelor's degree in electronic engineering and the PhD degree in electrical engineering from Polytechnic where he is currently a tenured assistant professor of human computer interaction in the Department of Electrical and Information Engineering and has also taught expert systems, medical informatics, and image processing. Since 1996, he has been working and investigating in the field of computer vision and image processing, neural networks, evolutionary algorithms, and hybrid expert systems. The main applications of his research are in real world, in biometry, in medicine, and recently in bioinformatics and systems biology. On July 2011, he was invited as a lecturer to the International School on Medical Imaging using Bio-inspired and Soft Computing-Miere (Spain) MIBISOC FP7-PEOPLE-ITN-2008. GA N. 238819—where he presented his research on Intelligent Tumors Computer Aided Early Diagnosis and Therapy: Neural Network and Genetic Algorithms frameworks. He won the Best Paper Award at the International Conference on Intelligent Computing held in Shanghai (ICIC 2008), and he was program chair of ICIC 2009, publication chair of ICIC 2010, tutorial chair of ICIC 2011, publication chair of ICIC 2012 and ICIC 2013, award committee chair of ICIC 2014, special issue chair of ICIC 2015, and general chair of HMISS 2015.

M. Michael Gromiha received the PhD degree in physics from Bharathidasan University, India, and served as the STA fellow, RIKEN researcher, research scientist, and senior scientist with the Computational Biology Research Center, AIST, Japan till 2010. Currently, he is working as a professor with the Indian Institute of Technology (IIT) Madras, India. His main research interests include structural analysis, prediction, folding, and stability of globular and membrane proteins, protein interactions, and the development of bioinformatics databases and tools. He has published more than 200 research articles, 40 reviews, six editorials, and a book entitled *Protein Bioinformatics: From Sequence to Function* by Elsevier/Academic Press. His papers received more than 9,000 citations and has a h-index is 52. He is an associate editor of *BMC Bioinformatics* as well as an editorial board member of *Scientific Reports*, *Biology Direct*, and the *Journal of Bioinformatics and Computational Biology*, *Genes and Current Computer Aided Drug Design*. He has received several awards including the Oxford University Press Bioinformatics prize, Okawa Science Foundation Research Grant, Young Scientist Travel awards from ISMB, JSPS, AMBO, ICTP etc., Best Paper Award at ICIC2011, ICTP Associateship Award, ICMR International Fellowship for Senior Biomedical Scientists, INSA Senior Scientist Award, Best Paper Award in Bioinformatics by the Department of Biotechnology, India, Institute Research and Development Award at IIT Madras, and the Outstanding Performance Award from Initiative for Parallel Bioinformatics (IPAB), the Tokyo Institute of Technology, Japan. He is a member of the National Academy of Sciences, India.

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