

Guest Editorial: Application and Development of Bioinformatics

Yi-Ping Phoebe Chen

BIOINFORMATICS and Computational Biology comprises the application and development of data theoretical and analytical approaches, computational simulation methods, and mathematical modeling to the study of biological and biomedical systems. In this special section, five papers in their significantly extended versions were selected from the papers presented at the 10th Asia Pacific Bioinformatics Conference (APBC2012). These papers show recent research in bioinformatics and computational biology consisting of peptide identification, gene regulatory networks, protein interaction networks, and signal transduction cascades or pathways. These papers have shown great collaboration and conscientious thinking throughout the complex and challenging bioinformatics and computational biology experiments.

In "QuickVina: Accelerating AutoDock Vina Using Gradient-Based Heuristics for Global Optimization," Stephanus Daniel Handoko, Xuchang Ouyang, Chinh Tran To Su, Chee Keong Kwoh, and Yew Soon Ong studied accelerating autoDock Vina using gradient-based heuristics for global optimization. They proposed to further improve the local search algorithm of Vina by the prevention of some points from undergoing the local search.

In "Improving X!Tandem on Peptide Identification from Mass Spectrometry by Self-Boosted Percolator," Pengyi Yang, Jie Ma, Penghao Wang, Yunping Zhu, Bing B. Zhou, and Yee Hwa Yang studied improving X!Tandem on peptide identification from mass spectrometry by self-boosted percolator. They proposed a self-boosted percolator for postprocessing X!Tandem search results. They improved the performance through multiple boost runs, which enabled more PSM identifications without sacrificing false discovery rate (FDR).

In "CEDER: Accurate Detection of Differentially Expressed Genes by Combining Significance of Exons Using RNA-Seq," Lin Wan and Fengzhu Sun learned of an accurate detection of differentially expressed genes by combining the significance of exons using RNA-Seq, widely used in transcriptome studies and the detection of differentially expressed genes (DEGs) between two classes

of individuals. They proposed developing a novel program, termed CEDER, to detect DEGs accurately.

In "How Little Do We Actually Know? On the Size of Gene Regulatory Networks," Richard Röttger, Ulrich Rückert, Jan Taubert, and Jan Baumbach studied the size of gene regulatory networks. They proposed predicting the sizes of the whole-organizing regulatory networks of seven species. It was concluded that they had lacked substantial understanding of fundamental molecular control mechanism on a large scale.

In "A Comparative Assessment of Ranking Accuracies of Conventional and Machine-Learning-Based Scoring Functions for Protein-Ligand Binding Affinity Prediction," Hossam M. Ashtawy and Nihar R. Mahapatra proposed exploring a range of novel SFs, employing different machine-learning approaches in conjunction with a variety of physicochemical and geometrical features characterizing protein-ligand complexes. SFs, which has a limited ranking accuracy, has been a major roadblock toward cost-effective drug discovery.

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Guest Editor



Yi-Ping Phoebe Chen received the BInfTech degree with first class honours and the PhD degree in computer science (bioinformatics) from the University of Queensland. She is a professor and chair and director of research in the Department of Computer Science and Computer Engineering, La Trobe University, Melbourne, Australia. Prof. Chen is the chief investigator of the ARC Centre of Excellence in Bioinformatics. She is currently working on knowledge discovery technologies and is especially interested in their application to genomics and biomedical science. Her research focus is to find the best solutions for mining, integrating, and analyzing complex data structure and functions for scientific and biomedical applications. She has been working in the area of bioinformatics, health informatics, multimedia databases, query system, and systems biology, has coauthored more than 180 research papers, with many published in top journals and conferences. She is steering committee chair of the Asia-Pacific Bioinformatics Conference (founder) and the International Conference on Multimedia Modelling. She has been on the program committees of more than 100 international conferences, including top ranking conferences such as ICDE, ICPR, ISMB, CIKM, etc. More information about her can be found at <http://homepage.cs.latrobe.edu.au/ypchen/index.htm>.

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