Guest Editorial for ACM BCB

Tamer Kahveci and Mona Singh

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It is our great pleasure to present this special section of the *IEEE/ACM Transactions on Computational Biology and Bioinformatics*. The special section includes nine papers, which were invited from the ACM Conference on Bioinformatics, Computational Biology and Biomedicine (ACM BCB) in 2012. ACM BCB is the flagship conference of the ACM SIG on Bioinformatics, Computational Biology and Biomedical Informatics (SIGBio). In total, 159 papers were submitted to the ACM BCB conference in 2012, among which 33 were accepted as regular papers. Of these, nine were invited for the special section. These papers were significantly extended from their earlier versions and went through a separate revision process. These papers cover a broad spectrum of applications, and have great potential to further bioinformatics and computational biology research.

In "Nonoverlapping Clone Pooling for High-Throughput Sequencing," Reginaldo M. Kuroshu considered the problem of splitting a given set of clones whose locations on the genome is known into independent subsets of clones such that no two clones in the same subset overlap on the genome. The author formulates this as a graph coloring and bin packing problem, both of which are well studied in the literature.

In "Improved Multiple Sequence Alignments Using Coupled Pattern Mining," K.S.M. Tozammel Hossain, Debprakash Patnaik, Srivatsan Laxman, Prateek Jain, Chris Bailey-Kellogg, and Naren Ramakrishnan developed a method named ARMiCoRe to align a given set of sequences which can identify and match couplings. A coupling is a pair of sequence positions whose values depend on each other across input sequences.

In "Reverse Engineering Molecular Hypergraphs," Ahsanur Rahman, Christopher L. Poirel, David J. Badger, Craig Estep, and T.M. Murali propose to use hypergraphs to describe gene networks, thereby enabling greater expression power to encompass the topology of interactions among more than two genes.

In "Stochastic Model Simulation Using Kronecker Product Analysis and Zassenhaus Formula Approximation," Mehmet Umut Caglar and Ranadip Pal describe uncertainty in gene regulatory networks using a stochastic model. They develop a new approach that reduces the cost of computing the stochastic master equation significantly by rewriting the reaction matrix as the sum of a set of very sparse matrices.

In "Coalescent-Based Method for Learning Parameters of Admixture Events from Large-Scale Genetic Variation Data," Ming-Chi Tsai, Guy Blelloch, R. Ravi, and Russell Schwartz aim to compute the parameters of admixture events explaining evolutionary histories from genetic variation data. They develop a novel method, named CLEAX, to compute these parameters using a coalescent-based inference model.

In "Quantitative Analysis of Live-Cell Growth at the Shoot Apex of *Arabidopsis thaliana*: Algorithms for Feature Measurement and Temporal Alignment," Oben M. Tataw, G. Venugopala Reddy, Eamonn J. Keogh, and Amit K. Roy-Chowdhurry build a framework to study live image data of growth features of organ primordia. They build a parameter-free landscape matching algorithm, named LAM-M, which is robust to noise and outliers in the input data.

In "Probabilistic Search and Energy Guidance for Biased Decoy Sampling in Ab initio Protein Structure Prediction," Kevin Molloy, Sameh Saleh, and Amarda Shehu explore the relationship between underlying energy functions and the sampling resolution of the search for ab-initio protein structure prediction. They focus on the Rosetta and AMW energy functions.

In "Expanded Explorations into the Optimization of an Energy Function for Protein Design," Yao-ming Huang and Christopher Bystroff study the suitability of several objective functions and energy functions for protein structure design.

In "Isolating Influential Regions of Electrostatic Focusing in Protein and DNA Structure," Seth Blumenthal, Yisheng Tang, Wenjie Yang, and Brian Y. Chen build geometric methods and a statistical model to locate large electrostatic focusing regions in biological molecules. They demonstrate the accuracy of their algorithm on a large collection of protein-DNA complexes.

As guest editors of this special section, we would like to thank the contributing authors, the ACM BCB 2012 program committee, the reviewers who reviewed the journal version of the papers for *TCBB*, and *TCBB* editorial staff for their invaluable contribution.

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Mona Singh received the AB and SM degrees in computer science from Harvard University, and the PhD degree in computer science from the Massachusetts Institute of Technology (MIT), Cambridge, Massachusetts. She is on the faculty at Princeton University, New Jersey, where she is a professor of computer science in the Computer Science Department and the Lewis-Sigler Institute for Integrative Genomics. She did postdoctoral work at the Whitehead Institute for Biomedical Research, Cambridge, Massachusetts. Her group develops computational methods for analyzing cellular networks, predicting specificity in protein interactions, and functionally characterizing proteins using sequence, structure and network approaches.