Data Mining in Bioinformatics: Selected Papers from BIOKDD

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BIOINFORMATICS is the science of managing, mining, and interpreting information from observations of biological processes. Various genome projects have contributed to an exponential growth in DNA and protein sequence databases. In the postgenome era, advances in high-throughput technology such as microarrays and mass spectrometry have further created the fields of functional genomics and proteomics, in which one can monitor quantitatively the presence of multiple genes, proteins, metabolites, and compounds in a given biological state.

Data mining approaches are ideally suited for bioinformatics. The ongoing influx of these data, the presence of biological signals despite high data noises, and the gap between data collection and knowledge extraction have collectively created new and exciting opportunities for data mining researchers in this field. The extensive availability of open-access biological databases has created both challenges and opportunities for developing novel knowledge discovery and data mining methods specific to molecular biology. While tremendous progress has been made over the years, many of the fundamental problems in bioinformatics, such as protein structure prediction, protein-ligand interactions, molecular pathway mapping, and gene regulatory network modeling, are still open. Many of the current research problems are comprehensively covered in a recent book by Chen and Lonardi [1]. Data mining will play essential roles in understanding these fundamental problems and developing novel therapeutic/diagnostic solutions in post-genome medicine.

To provide avenues to data mining researchers active in bioinformatics, we organized the 2008 International Workshops on Data Mining in Bioinformatics (BIOKDD), held 24-27 August in Las Vegas, NV (http://bio.informatics.iupui.edu/biokdd08/). In this issue of *TCBB*, we present two extended papers chosen from nine peer-reviewed papers originally presented at the workshop. The two papers were among nine top ranked papers with the highest peer review scores from more than 30 papers received at the BIOKDD workshop. They have been further refereed according to the *TCBB* manuscript submission standards: each invited paper was reviewed by three external referees and went through one or two rounds of revisions. In the end, two out of the four invited papers were included for publication.

The two contributions appearing in this special section are "Molecular Function Prediction Using Neighborhood Features" by Petko Bogdanov and Ambuj K. Singh and "GPD: A Graph Pattern Diffusion Kernel for Accurate Graph Classification with Applications in Cheminformatics" by Aaron Smalter, Jun Huan, Yi Jia, and Gerald Lushington. Bogdanov and Singh describe a framework for predicting functional annotation in molecular interaction networks. Contrary to the popular assumption that genes with similar functions are topologically close in interaction networks, the authors held a different view—genes with similar functions share similar annotation patterns in their network neighborhood independent of their distance in the network. This led the authors to classify and subsequently infer gene functions based on network neighborhood. Their approach appears to be more robust against noise and to be more adaptable be integrated with homology information. Smalter et al. describe a new computational framework for chemical structure comparisons and database search, based on the new notion of graph pattern diffusion kernel. Their approach allows the discovery and labeling of frequent graph patterns in a database of chemical structures. It represents a significant novel development for the interdisciplinary research community that aims to support chemical biology.

In closing, we would like to thank all of the contributing authors, the reviewers, and the staff of *TCBB* for the support offered during this project.

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[1] J. Chen and S. Lonardi, *Biological Data Mining.* Chapman & Hall/CRC, 2010.

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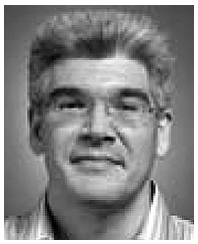

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