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Title	<Bioinformatics Center>Mathematical Bioinformatics
Author(s)	
Citation	ICR annual report (2011), 18: 62-63
Issue Date	2011
URL	http://hdl.handle.net/2433/154944
Right	
Type	Departmental Bulletin Paper
Textversion	publisher

Kyoto University

Bioinformatics Center
– Mathematical Bioinformatics –

http://www.bic.kyoto-u.ac.jp/takutsu/index.html

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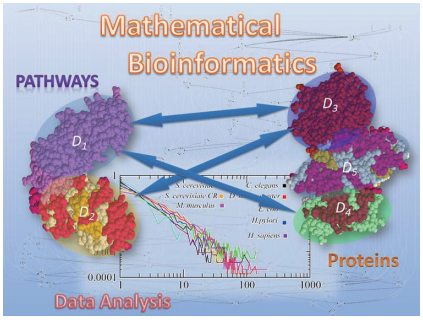
Assoc Prof CAPKOVIC, Frantisek	Institute of Informatics Slovak Academy of Sciences, Slovenská republika, 2 June
Prof ZHOU, Huarong	Chinese Academy of Sciences, China, P.R., 13 September
Dr SONG, Jiangning	Monash University, Australia, 12 December 2011–27 January 2012

Scope of Research

Due to rapid progress of the genome projects, whole genome sequences of organisms ranging from bacteria to human have become available. In order to understand the meaning behind the genetic code, we have been developing algorithms and software tools for analyzing biological data based on advanced information technologies such as theory of algorithms, artificial intelligence, and machine learning. We are recently studying the following topics: systems biology, scale-free networks, protein structure prediction, inference of biological networks, chemo-informatics, discrete and stochastic methods for bioinformatics.

KEYWORDS

Scale-free Networks
Boolean Networks
Grammar-based Compression
RNA Secondary Structures
Chemical Graphs



Selected Publications

Akutsu, T.; Fukagawa, D.; Takasu, A.; Tamura, T., Exact Algorithms for Computing Tree Edit Distance between Unordered Trees, *Theoretical Computer Science*, **421,** 352-364 (2011).

Nacher, J. C.; Akutsu, T., On the Degree Distribution of Projected Networks Mapped from Bipartite Networks, *Physica A*, **390,** 4636-4651 (2011).

Imada, T.; Ota, S.; Nagamochi, H.; Akutsu, T., Efficient Enumeration of Stereoisomers of Outerplanar Chemical Graphs Using Dynamic Programming, *Journal of Chemical Information and Modeling*, **51,** 2788-2807 (2011).

Hayashida, M.; Kamada, M.; Song, J.; Akutsu, T., Conditional Random Field Approach to Prediction of Protein-Protein Interactions Using Domain Information, *BMC Systems Biology*, **5 (Suppl. 1),** S8 (2011).

Sato, K.; Kato, Y.; Hamada, M.; Akutsu, T.; Asai, K., IPknot: Fast and Accurate Prediction of RNA Secondary Structures with Pseudoknots Using Integer Programming, *Bioinformatics*, **27,** i85-i93 (2011).

Discriminative Random Field Approach to Prediction of Protein Residue Contacts

For understanding constructions and evolution of biomolecular networks and cellular systems, it is important to analyze molecular recognition and specific interactions of proteins. Many investigations have been conducted to analyze interactions and contacts between residues. It is supported that residues at interacting sites have co-evolved with those at the corresponding residues in the partner protein to keep the interactions between the proteins. Therefore, mutual information (MI) between residues calculated from multiple sequence alignments of homologous proteins is considered to be useful for identifying contact residues in interacting proteins.

In our previous work, we proposed a prediction method for protein-protein interactions using mutual information and conditional random fields (CRFs), and confirmed its usefulness. The discriminative random field (DRF) is a special type of CRFs, and can recognize some specific characteristic regions in an image. Since the matrix consisted of mutual information between residues in two interacting proteins can be regarded as an image, we propose a prediction method for protein residue contacts using DRF models with mutual information. To validate our method, we perform computational experiments for several interactions between Pfam domains. The results suggest that the proposed DRF-based method with MI is useful for predicting protein residue contacts compared with that using the corresponding Markov random field (MRF) model.

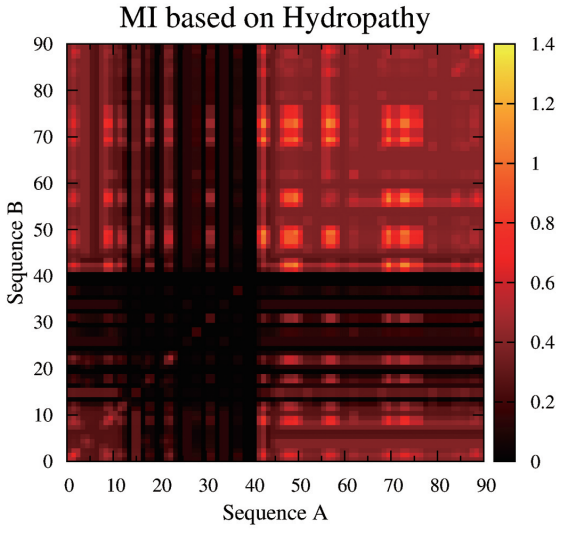


Figure 1. Mutual information between residues.

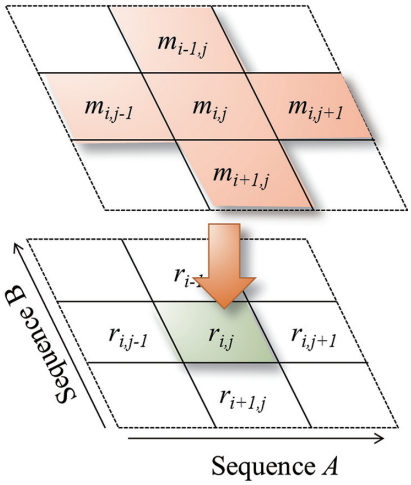


Figure 2. Discriminative random field model for protein residue interactions.

Computing Impact Degrees for Multiple Reactions in Metabolic Networks with Cycles

The impact degree is a measure of the robustness of a metabolic network against deletion of single or multiple reaction(s). Although such a measure is useful for mining important enzymes/genes, it was defined only for networks without cycles. In this work, we extend the impact degree for metabolic networks containing cycles and develop a simple algorithm to calculate the impact degree. Furthermore we improve this algorithm to reduce computation time for the impact degree by deletions of multiple reactions. We applied our method to the metabolic network of *E. coli*, that includes reference pathways, consisting of 3281 reaction nodes and 2444 compound nodes, downloaded from KEGG database, and calculate the distribution of the impact degree. The results of our computational experiments show that the improved algorithm is 18.4 times faster than the simple algorithm for deletion of reaction-pairs and 11.4 times faster for deletion of reaction-triplets. We also enumerate genes with high impact degrees for single and multiple reaction deletions.

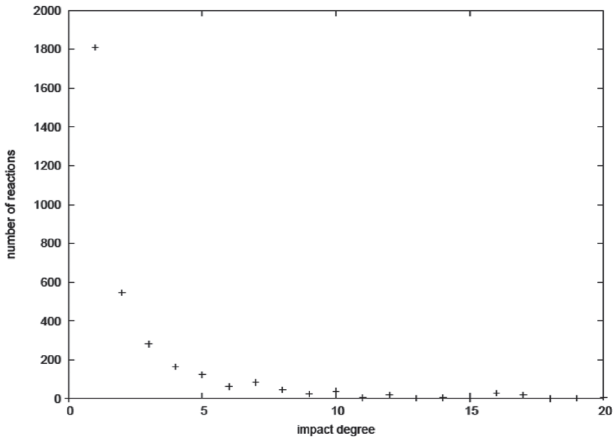


Figure 3. Distribution of impact degree for single-reaction deletion. The average impact degree is 2.651. The maximum impact degree is 55.