Bioinformatics Center
- Biological Information Network -

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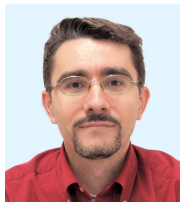

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Visitors

Prof HALLDORSON, Magnus	University of Iceland, 21 April, 2003
Dr VERT, Jean-Philippe	Ecole des Mines de Paris, 24 October - 8 November, 2003
Mr CUTURI, Marco	Ecole des Mines de Paris, 27 October - 31 October, 2003
Mr MAHE, Pierre	Ecole des Mines de Paris, 1 December - 12 December, 2003

Scope of Research

Due to rapid progress of the genome projects, whole genome sequences of many organisms and a draft of human genome sequence have been already determined. But, the determination of the whole genome sequences does not mean the end of analysis of genetic code. In order to understand the meaning behind the genetic code, we have been developing algorithms for analyzing proteomics data and genomics data. Recently, we focus on the following topics: protein-protein interaction, remote homology detection, and cheminformatics.

Research Activities (Year 2003)

Presentations

Efficient extraction of mapping rules of atoms from enzymatic reaction data, Akutsu T, The 7th Annual Int'l Conf. on Research in Computational Molecular Biology, 12 April.

Optimization problems and metaheuristics in bioinformatics, Akutsu T, The 5th metaheuristics Int'l Conf., 28 August.

Performance analysis of a greedy algorithm for inferring Boolean functions, Fukagawa D, Akutsu T, The 6th Int'l Conf. on Discovery Science, 18 October.

Inferring strengths of protein-protein interactions from experimental data using linear programming, Hayashida M, Ueda N, Akutsu T, European Conf. on Computational Biology, 28 September.

Computational and statistical methods in bio-informatics, Akutsu T, The 14th Int'l Symp. Methodologies for Intelligent Systems, 28 October.

Grants

Akutsu T, Miyano S, Ueda N, Algorithms for finding common patterns in bioinformatics, Grant-in-Aid for Scientific Research (C) (2), 1 April 2001 - 31 March 2005.

Akutsu T, Genome information science (a member of the project), Grant-in-Aid for Scientific Research Priority Areas (C) , 1 April 2000 - 31 March 2005.

Ueda N, Statistical language models that generate a pair of sequences for sequence analysis, Grand-in-Aid for Encouragement of Young Scientists, 1 April 2003 - 31 March 2006.

Inferring strengths of protein-protein interactions with linear programming

Since protein-protein interaction plays a key role in any cellular processes, several computational methods have been proposed for inference of protein-protein interaction. They consider that the interaction is represented as binary, i.e., whether two proteins interact or not. However a data set of the ratios (strengths) of interaction between two proteins becomes available since multiple experiments of the interactions for the same protein pairs were performed recently in practice. We then develop a new method to infer the strength of the interaction with linear programming. Experimental results show that it outperforms existing methods on the data set of the ratios of interactions.

1. Hayashida M, Ueda N, Akutsu T, Inferring strengths of protein-protein interactions from experimental data using linear programming, Bioinformatics, 19, supplement, pp. ii58 - ii65 (2003).

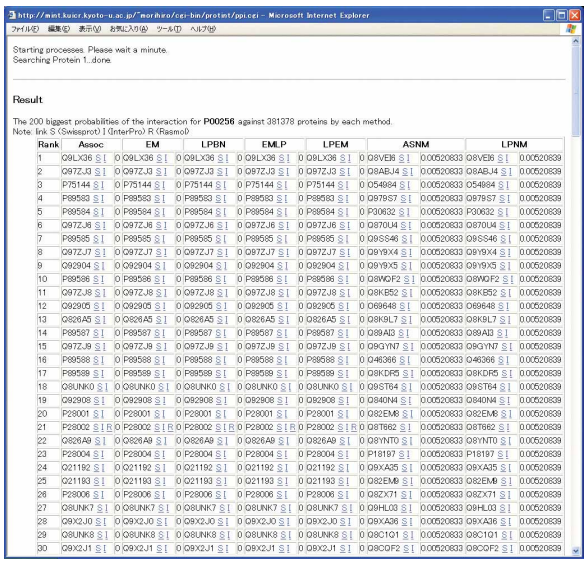

Figure 1. A system for inferring strengths of protein-protein interactions.

Efficient extraction of mapping rules of atoms from enzymatic reaction data

Extraction of mapping rules of atoms from enzymatic reactions is useful for drug design, simulation of tracer experiments and consistency checking of pathway databases. Most of previous methods for this problem are based on maximal common subgraph algorithms. We then propose a novel approach based on graph partition and graph isomorphism. The results of computational experiments suggest that the proposed method is useful in many cases.

1. Akutsu T, Efficient extraction of mapping rules of atoms from enzymatic reaction data, 7th Annual Int'l Conf. on Research in Computational Molecular Biology, pp. 1 - 8 (2003).

Protein homology detection using string alignment kernels

Several methods have been developed recently for remote homology detection for protein sequences using support vector machines (SVMs), and we developed one method called SVM-SW. To achieve higher accuracy of the detection, we improved the method by designing a new kernel function which measures similarity between two protein sequences with the local alignment. The designed kernel function and SVMs (Fig. 2) performed better than several existing methods on a benchmark data set.

Figure 2. A system for protein remote homology detection using string kernels.