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ワークショップ参加レポート

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Title: Minimum Reaction Cuts of Metabolic Networks Under a Boolean Model

Workshop report：

In this work, we consider the problem of, given a metabolic network, a set of source compounds and a set of target compounds, finding a minimum size reaction cut, where a Boolean model is used as a model of metabolic networks. The problem has potential applications to measurement of structural robustness of metabolic networks and detection of drug targets. We develop an integer programming-based method for this optimization problem. In order to cope with cycles and reversible reactions, we further develop a novel integer programming (IP) formalization method using a feedback vertex set (FVS). When applied to an E. coli metabolic network consisting of Glycolysis/Glyconeogenesis, Citrate cycle and Pentose phosphate pathway obtained from KEGG database, the FVS-based method can find an optimal set of reactions to be inactivated much faster than a naive IP-based method and several times faster than a flux balance-based method. We also confirm that our proposed method works even for large networks and discuss the biological meaning of our results.

In the poster session of IBSB2009, there were an useful discussion on the application of our work. In this discussion, the idea of utilizing the notion of substructures of compounds was proposed. This idea is based on that every reaction in metabolic networks can be regarded as composition and decomposition of substructures of compounds. By combining this idea and our work, it is possible to find substructures of compounds whose deletion impact many reactions and compounds. Such substructures should be important from the view point of biology. Alignment for sequences of genes related to such substructures may output DNA sequences with biological importance. To conduct the study based on the above idea, it is necessary to extend metabolic networks by adding substructures of compounds to the ordinary network. Such extension will be one of our future works.

In addition to the above discussion on the topic related the title of our poster, there were discussion with Nils Christian, who visited Kanehisa laboratory of Kyoto university last year. His talk on IBSB2009 was based on our collaborating work on nutrient profiles. In this work, I play a role on conducting computer experiment with support vector machines. I also conducted recursive feature elimination before the conference, but I failed to obtain reasonable results on this part. However, the discussion with Christian and Prof. Akutsu turned out my misunderstanding on this part. I will be able to modify my program and will obtain new results on this work.