第 10 回 2013 年 1 月 11 日（金）15:40 ~ 16:30

Inference of Gene Regulatory Network by Structural Equation Modeling

構造方程式モデリングによる遺伝子ネットワーク推定

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The control of gene expression is an important regulatory system for living cells. Inferring a gene regulatory network is one of the useful methods to clarify the regulatory mechanisms. Recently, I developed a new statistical approach, based on SEM in combination with stepwise factor analysis, to infer the protein-DNA interactions for gene transcriptional control from only the gene expression profiles, in the absence of protein information. Although the inferred model had a simple hierarchy, my development approach was considered to be useful for distinguishing transcription factors' regulation from other transcriptional regulation.

In this lecture, I'll show you the recent investigations of SEM approach for inferring more complicated gene regulatory networks.

Keywords: Structural Equation Modeling, Network Inference, Expression Profile

第 10 回 2013 年 1 月 11 日（金）14:50 ~ 15:40

State transition of living cells and time series analyses

細胞の状態変化と時系列データ解析

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Several mathematical models based on systems of ordinary differential equations (ODEs) have been proposed for the representation of RNA interference (RNAi) dynamics. These consist of equations for molecular elements involved in RNAi, and so there are many real-value parameters that must be optimized in order to identify the models. They also have many `hidden variables', which cannot be observed directly by experiment. Calculation of the values or profiles of the hidden variables is generally difficult, if not impossible, and identification of the ODE models is also quite difficult in this situation.

We show that the simplified logistic Lotka-Volterra model, which is one of the most well-established ODE models for biological and biochemical phenomena, can represent RNAi dynamics as a predator-prey system that models the apoptosis of HeLa cells by small interfering RNA (siRNA). Although there is a hidden variable, the values can be determined, or made visible as dynamic profiles of RNA decomposing effects of siRNAs. Model parameters correlate highly with the total effect of the siRNA.

Keywords: time series analysis, state transition, gene expression analysis, statistical models, optimization

第 11 回 2013 年 1 月 18 日（金）14:50 ~ 15:40

An exhaustive similarity search of known and putative ligand binding sites in proteins

タンパク質の既知及び推定基質結合部位の網羅的類似探索

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We proposed an ultrafast alignment-free method for comparing huge number of protein-ligand binding sites, in which binding sites are mapped as vectors onto a high-dimensional feature space based on their physicochemical and geometrical properties. Once binding sites are represented as bit strings, called structural sketches, which is obtained by random projections of the vectors, a multiple sorting method is applied to the enumeration of all similar pairs in terms of the Hamming distance. With 3.4 million known and potential ligand binding sites, the proposed method found 24 million similar binding site pairs. Performing such a comprehensive comparison has been demonstrated to be useful for annotation of protein functions.

Keywords：protein-ligand interactions, similarity search, functional sites, database

第 11 回 2013 年 1 月 18 日（金）15:40 ~ 16:30

Detection of molecular candidates responsible for phenotype changes by computational analysis of omics data

オミックスデータ数理解析による表現型変化の要因となる分子候補の検出

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Recently, we proposed a new approach for analyzing omics data. Our approach is distinctive from previous ones. In contrast to previous approaches in which molecular data are unified by several mathematical ways to describe phenotype data, from “bottom-up” view point, we adopt a “top-down” approach, by focusing on the phenotype difference between samples, rather than those between molecular data. The performance of our approach was examined for the progression data from diabetes rats and the proteomics data from lung cancer cell lines, and these analyses revealed a set of molecular functions more clearly, in comparison with those by a standard “bottom-up” approach.

Keywords : phenotype, omics data, computational systems biology

第 12 回 2013 年 1 月 25 日（金）14:50 ~ 16:30

Representation and interpretation of biological data

生命科学データの表現と解釈

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Recent technological advances have enabled life scientists to conduct massively parallel experiments and access an abundance of data sets publicly available on the Internet. As a consequence, modern life science is facing with a severe bottleneck in the step of generating interpretable hypotheses or "stories" from the big and multidisciplinary data. In this seminar, I will present some bioinformatics approaches for representing large and complicated biological data and organizing knowledge in distant fields effectively.

Keywords : Data representation, visualization, evolution, biological networks, literature