CMRU Symposium

Mathematical Models and Simulations for Real World Networks

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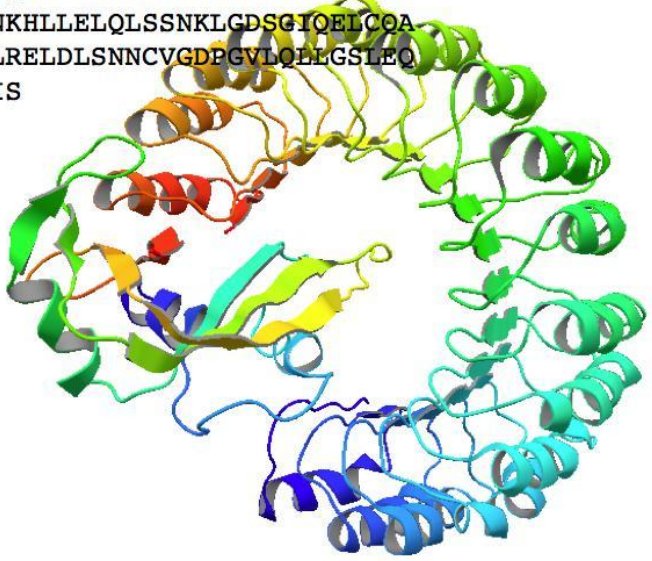

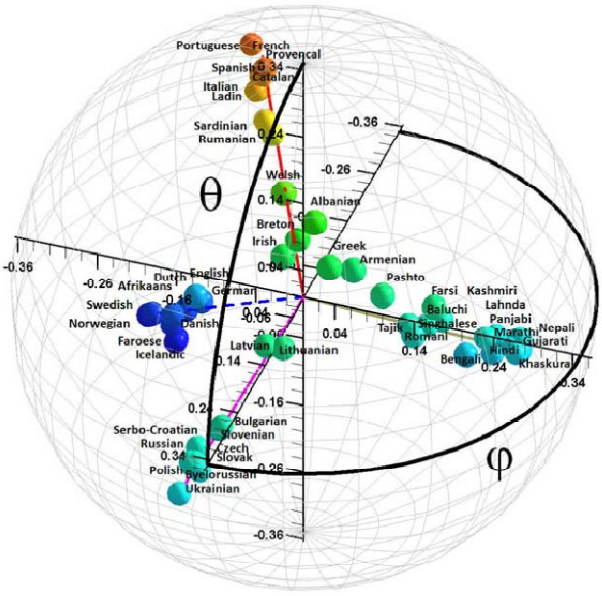

February 23, 2011

Graduate School of Information Sciences

Tohoku University

PROGRAM

1330 *Opening Address*

Michitaka Kameyama

Dean, Graduate School of Information Sciences, Tohoku University

1340-1430

Inhomogeneous Random Graph Models and Generalized Percolation and Epidemic Processes

Philippe Blanchard

Faculty of Physics and ZiF, University of Bielefeld

1450-1540

Information Theoretic Background of Statistical Potentials of Protein Structures

Matsuyuki Shirota

Graduate School of Information Sciences, Tohoku University

1600-1650

Learning Multiple Belief Propagation Fixed Point for Real Time Road Traffic Inference

Cyril Furtlehler

Institut National de Recherche en Informatique et Automatique (INRIA), Sacley, TAO Project-Term

1700 *Closing*

CMRU The *Collaborative Mathematics Research Unit* was just founded in January 2011 as part of the Graduate School of Information Sciences (GSIS), Tohoku University. The CMRU aims at contributing to the development of collaborative study of mathematics and other fields of science, particularly, information science, biological and life science, social and environmental science, and others.

ABSTRACTS

Inhomogeneous Random Graph Models and Generalized Percolation and Epidemic Processes

Philippe Blanchard (Faculty of Physics and ZiF, University of Bielefeld)

We review the theory of inhomogeneous random graph models, Cameo graphs (Blanchard-Krüger 2004) and BJR graphs (Bollobas-Janson-Riordan 2005) and the generalized epidemic process (GEP) formalism including local dynamics and global mean field dynamics and discuss their main properties: phase transitions, connection to threshold percolation, communication index and all that. We introduce different GEP models to describe the spreading of different social processes and "diseases" like corruption, knowledge, innovation, opinion, terrorism ....

Information Theoretic Background of Statistical Potentials of Protein Structures

Matsuyuki Shirota (Graduate School of Information Sciences, Tohoku University)

The prediction of the three-dimensional structure of a protein from its amino acid sequence is a challenging task in computational biology. For this task, various model structures are generated for a given amino acid sequence, and the quality of these models must be evaluated to select the most reliable one as the prediction result. One major group of such model evaluation methods is the statistical potential, which is based on the conformational preferences observed among the known protein structures in the Protein Data Bank (PDB). We discuss the information theoretic background of the statistical potentials both in terms of constructing them from PDB and in terms of using them to evaluate model structures. In the former part, the reference state must be defined to quantify the significance of the observed occurrence of the conformations. We demonstrate that apparently arbitrary choices of the reference states result in the differences in the accuracy in model evaluation due to the changes in the physical properties of the statistical potentials such as hydrophobicity and attractiveness. In the latter part, we reformulate the statistical potentials as the absolute quality scores, i.e. the scores of different proteins can be compared with each other. We first recast the statistical potential as the difference between the Kullback-Leibler divergence from a model structure to the native state and that to the reference state. We then show that statistical potentials can evaluate the absolute quality of models of various native-likeness with respect to the native states and the reference states, although these potentials are developed by using only the data set of native structures. These analyses shed light to the information theoretic aspect of statistical potentials that the native-like state of a model structure is evaluated with respect to the native structures in the PDB.

Learning Multiple Belief Propagation Fixed Point for Real Time Road Traffic Inference

Cyril Furtlehner (Institut National de Recherche en Informatique et Automatique (INRIA), Sacley, TAO Project-Term)

We consider the generic problem of inferring present and future configurations of a complex system, based on partial present-time observations in addition to past observations of its behavior. To address this question we develop a method based on the "loopy belief propagation" algorithm, as a surrogate to an exact Markov Random Field modelling, computationally too expensive for large scale systems. A prior information composed of correlations among a large set of N variables, is encoded into a graphical model; this encoding is optimized with respect to an approximate decoding procedure, which is used to infer hidden variables from an observed subset. We focus on the situation where the underlying data have many different statistical components, representing a variety of independent patterns. We define a model able to associate a belief propagation fixed point to each component of the underlying probabilistic mixture. Asymptotic analysis reveal an exact connection with some Hopfield model at finite temperature and steady state, when the number of mixture components is proportional to the number of variables. We then discuss the relevance of this results to the problem of reconstructing and predicting traffic states based on floating car data and show some experiments based on artificial and real data.

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東北大学情報科学研究科重点研究プロジェクト「多様なセンサー情報を融合した道路交通流のナウキャストとフォアキャスト」
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