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Statistical Physics of Networks, Information and Complex Systems

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Overview

In this project we explore the mathematical methods and concepts of statistical physics that are finding abundant applications across the scientific and technological spectrum from soft condensed matter systems and bio-informatics to economic and social systems. Our approach exploits the considerable similarity of concepts between statistical physics and computer science, allowing for a powerful multi-disciplinary approach that draws its strength from cross-fertilization and multiple interactions of researchers with different backgrounds. The work on this project takes advantage of the newly appreciated connection between computer science and statistics and addresses important problems in data storage, decoding, optimization, the information processing properties of the brain, the interface between quantum and classical information science, the verification of large software programs, modeling of complex systems including disease epidemiology, resource distribution issues, and the nature of highly fluctuating complex systems. Common themes that the project has been emphasizing are (i) neural computation, (ii) network theory and its applications, and (iii) a statistical physics approach to information theory. The project's efforts focus on the general problem of optimization and variational techniques, algorithm development and information theoretic approaches to quantum systems. These efforts are responsible for fruitful collaborations and the nucleation of science efforts that span multiple divisions such as EES, CCS, D, T, ISR and P. This project supports the DOE mission in Energy Security and Nuclear Non-Proliferation by developing novel information science tools for communication, sensing, and interacting complex networks such as the internet or energy distribution system. The work also supports programs in Threat Reduction and Homeland Security.

Introduction

Breakthroughs in graph theory and in network theory, and the interactions of insights from statistical physics with classical information theory are enriching the breath and impact of information science and technology. The central role and sophistication of the computer tool, the power of its data-gathering and storing capabilities and the importance of the communication protocols governing the information-based economy motivated the laboratory to target information security as one of its focal points in its transformation to a capabilities laboratory. In addition, the increased computing power and the increased availability of stored data sets are opening up new avenues that require novel techniques to handle large data sets and optimize the computing technology. The CNLS-project 'statistical physics of information' targets the science that underpins central LANL efforts in information science and technology. Specifically, research that has been carried out in CNLS within the framework of this project contributes to the fundamental issues of (A) general optimization problems and variational approaches, (B) algorithm development, (C) networks, and (D) information theory approaches to quantum systems.

A. The general problem of optimization and variational approaches

Many important problems in molecular biology, epidemiology and other fields can be represented by random walks on large dimensional hyper-cubes. The states of the system are represented by strings of zeros and ones. For example, in an epidemiological model, a 1 at the i^{th} node may correspond to the i^{th} person being infected. Similarly, in a biochemical model, a 1 may correspond to the i^{th} methylation site being occupied by a methyl group. For a hyper cube of N dimensions, there are 2^N possible states. The master equation for this process may have dimension 2^N, but the interesting dynamics are typically much smaller in dimension. Under some reasonable assumptions, and with the right reduction and moment closure techniques, one can decompose this problem and solve or approximate the exact solution. With the exact solutions in hand, one can also observe that important quantities, such as the waiting time to go from all zeros to all ones, can be well approximated with relatively simple, well-known distributions - defined by parameters which one may be able to measure empirically from experimental data. We are developing this concept for application to biological systems.

Some of our work on statistical approaches to biological systems relates to the master equation approach for discrete state, continuous time Markov processes. Using projection techniques for finite elements allows one to significantly reduce the dimension of the master equation dynamics without prior knowledge of system characteristics (e.g., eigenvalues/eigenvectors). We have developed an algorithm that allows one to automatically (iteratively) find a good projection, which works well for a specified transient time. This reduction automatically averages (or removes) dynamics that are fast (or slow) in comparison with the time scale of interest. This could be a very cheap way to obtain such a timescale reduction. Some of this work was presented in a series of three lectures at the 2008 q-bio conference.

CNLS researchers have also explored the possibility of identifying parameters for stochastic processes based upon output distributions. Key findings include: the information in a probability distribution can enable a better system identification than mean behavior. For example, in the standard gene transcription and translation process, stochastic rates can be identified from the marginal distribution of proteins (with no direct observation of mRNA). This identification cannot be achieved through observation of the protein mean alone. Furthermore, transient data is essential for the identification of some system parameters - this could provide guidelines for experiment-based identification and even suggests simple fluorescence activated cell-sorting (FACS) and flow-cytometry experiments. This work will be presented at the 2009 IEEE Conference on Decision and Control.

The problem of optimization is a common theme in many areas of science, from computer science and information theory to engineering and statistical physics, as well as to biology or social sciences. Methods of optimization typically involve a large number of variables, e.g., particles, agents, cells or nodes, and a cost function depending on these variables, such as energy, measure of risk, or expense. A particularly challenging class of optimization problems is the so-called NP-complete problem, where the number of operations required to minimize the cost function scales exponentially or faster with system size. In many specific cases, however, even NP-complete problems may be easily solved. CNLS researchers are addressing the question of how to recognize if an NP-complete problem is typically hard, and what are the main reasons for this? Answering this question is crucial for developing new efficient algorithms for hard problems and for designing secure cryptographic systems. We use approaches from the physical theory of disordered systems, extending the so-called cavity method to discover new properties of the space of solutions in two of the most studied constraint satisfaction problems - random K-satisfiability and random graph coloring. We suggested a relation between the existence of the so-called frozen variables and the algorithmic hardness of a problem. Based on these insights, we introduced [Zdeborova & Mezard, 2008] a new class of problems that we call "locked constraint satisfaction." This class of problems is easily solvable, but from the algorithmic point of view these problems are even harder than the canonical K-satisfiability problems.

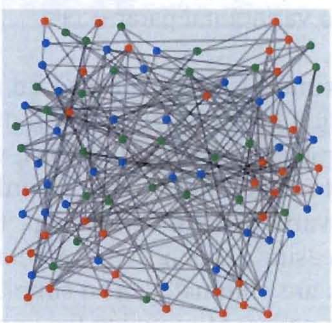


Fig. 1 Optimal coloring of a random graph.

CNLS researchers explored constrained minimization/optimization problems with non-commutative (matrix) variables, relevant to computational complexity of planar graphical models with constraints. We explained [Chertkov et al, 2008] the relationship between the dimer approach for planar graphical models and Belief Propagation/Loop Calculus approximations, indicating a new method for classifying the computational complexity of graphical models with constraints (loops). We also proved the localization property of special classes of orthogonal polynomials relevant in learning algorithms for high-dimensional data (e.g., image-recognition algorithms) [Teodorescu et al, 2008a, 2008b]. In information science work related to cold atom science, we showed how one can obtain quantum information processing with cold Fermi gases in the fast pairing regime [Teodorescu, 2009].

Graphical models (e.g., Markov random fields or Bayesian networks) provide compact representation of the joint probability distribution of large systems of random variables. Nodes of the graph represent random variables and edges denote interactions among variables. These models are widely used in science and engineering (e.g., statistical physics, image and signal processing, remote sensing, sensor networks, information theory). Owing to the intractability of optimal inference and estimation in general graphical models, there has been much research in recent years aimed at developing principled yet tractable approximate inference methods. Typical inference problems include computing the marginal distribution of each variable, computing the most probable joint configuration of all variables and computing the likelihood of a set of measurements of a subset of variables. All of these problems can be reduced to that of computing the partition function of the graphical model, which is a weighted sum over all configurations of the variables. We focus on estimating this quantity by computing upper bounds and then minimizing the upper-bound with respect to variational parameters.

We further develop a new variational approach to approximate inference based on an exact decimation (variable elimination) method for computing the partition function of a graphical model. Whereas the exact procedure becomes intractable in general graphs, we propose an inexact variational formulation. This entails introduction of a reduced-order representation of the effective potentials induced at each variable elimination step. By imposing constraints that the partition function is non-decreasing at each step, we obtain an upper bound on the partition function once all variables are eliminated. The simplest version of this approach involves passing messages between nodes. Minimizing the upper bound over all possible values of the messages (subject to inequality constraints which ensure that we maintain an upper-bound) results in a constrained convex optimization problem in the form of a geometric program, which is efficiently solved using interior-point methods.

B. Algorithm development

There are several combinatorial problems related to graphical models and networks for which no algorithms (even approximate approaches) are known. These problems exhibit a complexity that grows faster than exponential in the size of the problem description and they are known as NP-hard problems. Much of the current research in coding theory, as well as problems of interest to LANL such as network interdiction problems, fall in this category. This problem has several applications of interest to LANL such as nuclear non-proliferation, interception of smuggling activities, prevention of spread of infections, and computer network security (internet worms and bots). The general interdiction problem is especially difficult, since even a constant factor approximation is known to be NP-hard. CNLS researchers identified an important practical special case of the network interdiction problem, where reliable interdiction can be assumed to occur at some single edge (such as a border checkpoint or computer network firewall) along any network path of interest. For that case we provided an exact deterministic algorithm that runs in a time that is roughly quadratic in the size of the network and scales well to be useful in solving large network interdiction problems such as global transportation networks.

Other CNLS scientists specialize in the use of graphs/networks as a substrate for modeling knowledge, see Fig. 2. Although most of this work is at the symbolic level, recent applications in the PetaNet project at LANL led to an effort at the sub-symbolic level usually associated with artificial neural networks. Significant progress has been made in this area. In collaboration with University of Durham scientists, we have advanced our knowledge of formal logics thereby realizing a very significant, seemingly unseen, overlap between discrete walks on a graph and entailment in logic [Rodriquez & Geldart, 2009]. This joint work has lead to symbolic knowledge processing with directed labeled graphs and a technique we developed previously, known as grammar-based random walks (i.e., random walkers for labeled graphs). The work in this area has made impact on technology transfer through a copyright agreement with a local small business and with information categorization with the LANL Library.

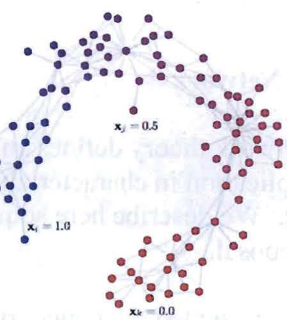


Fig. 2 Network model of dynamically distributed democracy.

Although information theory was developed by Claude Shannon in 1948 as a tool for calculating the maximum compression of data in communications, it has been applied to many other areas, especially statistical and dynamical systems with many degrees of freedom. Information quantities can be used to identify and classify correlations between variables, even in the absence of a model of their interactions. Also, the ability to process and react to information strongly influences the structure of many biological systems, such as neuronal or gene regulatory networks; therefore information theory is a natural framework for studying systems such as these. An example is two autonomous agents (say, mobile robots) that are searching for a source of radiation. A recent paper in Nature showed that searching based on maximizing information ("infotaxis") can be more effective than a standard gradient search. One of our current research themes is extending this idea to multiple, coordinated searchers. Preliminary results show that, using this formalism, it is possible to have synergetic coordination between multiple searchers and that deliberately synergetic motion can lead to more efficient searches. In Fig. 3, we show the synergy for an arrangement of searcher locations. The source (black dot) emits particles that have an angular correlation (2 particles are always emitted in opposite but random directions) and the location of one searcher (black star) is fixed. The grid shows the synergy (blue) or independence (white) of the arrangement as a function of positions for a second searcher. When the searchers are close together they are competing for the same particle (independence), but if the second searcher is near the source synergy is possible.

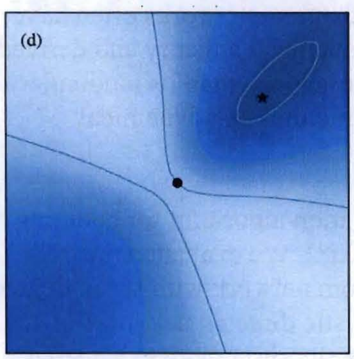


Fig. 3 Synergy for an arrangement of searcher locations.

C. Networks

Network theory defines an approach to understanding discrete graphs that has found application in characterizing social systems, internet connections, biological networks, etc. We describe here some of our work on networks that has emerged during this proposal.

We presented [Bettencourt et al, 2008] a general information theoretic approach for identifying functional sub-graphs in complex networks. We showed that the uncertainty in a variable can be written as a sum of information quantities, where each term is generated by successively conditioning mutual informations on new measured variables in a way analogous to a discrete differential calculus. The analogy to a Taylor series suggests efficient optimization algorithms for determining the state of a target variable in terms of functional groups of other nodes. We applied this methodology to electrophysiological recordings of cortical neuronal networks grown in vitro. Each cell's firing is generally explained by the activity of a few neurons. We identified these neuronal sub-graphs in terms of their redundant or synergetic character and reconstruct neuronal circuits that account for the state of target cells.

Previous work on undirected small-world networks established the paradigm that locally structured networks tend to have a high density of short loops. On the other hand, many realistic networks are directed. We investigated [Bianconi et al, 2008] the local organization of directed networks and found, surprisingly, that real networks often have very few short loops as compared to random models. We developed a theory and derived conditions for determining if a given network has more or less loops than its randomized counterparts. These findings carry broad implications for structural and dynamical processes sustained by directed networks.

In related work, CNLS researchers derived a Belief-Propagation algorithm for counting large loops in a directed network [Bianconi & Gulbahce, 2008]. We evaluated the distribution of the number of small loops in a directed random network with given degree sequence. We then applied the algorithm to a few characteristic directed networks of various network sizes and loop structures and compared the algorithm with exhaustive counting results where possible. We demonstrated that the algorithm is adequate in estimating loop counts for large directed networks and can be used to compare the loop structure of directed networks and their randomized counterparts.

We also systematically studied and compared damage spreading at the sparse percolation (SP) limit for random Boolean and threshold networks with perturbations that are independent of the network size N [Rohlfe et al, 2007]. This limit is relevant to information and damage propagation in many technological and natural networks. Using finite-size scaling, we identified a new characteristic connectivity K_s, at which the average number of damaged nodes, d, after a large number of dynamical updates, is independent of N. Based on marginal damage spreading, we determined the critical connectivity K_c^{sparse} (N) for finite N at the SP limit and showed that it systematically deviates from K_c , established by the annealed approximation, even for large system sizes. Our findings potentially explain the recent results obtained for gene regulatory networks and have important implications for the evolution of dynamical networks that solve specific tasks.

We also applied network theory to metabolic networks [Motter et al, 2008]. An important goal of medical research is to develop methods to recover the loss of cellular function due to mutations and other defects. Many approaches based on gene therapy aim to repair the defective gene or to insert genes with compensatory function. We proposed an alternative, network-based strategy that aims to restore biological function by forcing the cell to either bypass the functions affected by the defective gene, or to compensate for the lost function. Focusing on the metabolism of single-cell organisms, we investigated, using computational methods, mutants that lack an essential enzyme, and thus are unable to grow or have a significantly reduced growth rate. We showed that several of these mutants can be turned into viable organisms through additional gene deletions that restore their growth rate. In a rather counterintuitive fashion, this is achieved via additional damage to the metabolic network. Using flux balance-based approaches, see Fig. 4, we identified a number of synthetically viable gene pairs, in which the removal of one enzyme-encoding gene results in a non-viable phenotype, while the deletion of a second enzyme-encoding gene rescues the organism. The systematic network-based identification of compensatory rescue effects may open new avenues for genetic interventions.

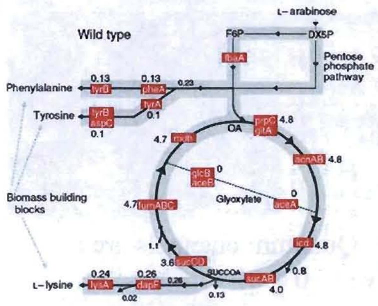


Fig. 4 Distribution of metabolic fluxes in the E.coli's TCA cycle.

In work [Lopez et al, 2007] that connects the statistical physics concept with complex networks, we studied the stability of network communication after removal of a fraction q=1-p of links under the assumption that communication is effective only if the shortest path between nodes i and j after removal is shorter than a ℓ_{ij} (a≥1) where ℓ_{ij} is the shortest path before removal. For a large class of networks, we found analytically and numerically a new percolation transition at $p_c = (K_o - 1)^{(1-a)/a}$, where $Ko = \langle k^2 \rangle / \langle k \rangle$ and k is the node degree. Above p_c , order N nodes can communicate within the limited path length a ℓ_{ij}, while below p_c , N^δ ($\delta < 1$) nodes can communicate. Our results should influence network design, routing algorithms, and immunization strategies, where short paths are most relevant.

D. Information theory approaches to quantum systems

The information carried by quantum particles differs fundamentally from the type of information flowing through today's computers and networks. "Quantum information", as it is called, exhibits surprisingly different behavior than the more familiar classical information. A deeper understanding of quantum information properties suggests dramatic and surprising prospects for a quantum-information architecture. Such an architecture would not only improve computational power, but would also establish unconditionally secure communication.

A basic concern for realizing quantum communication protocols is the protection of quantum information from noise. A noisy quantum process can be viewed as a communication channel. CNLS researchers made fundamental contributions to the theory of asymptotically perfect error correcting codes for point-to-point [Hayden et al, 2008] and network [Yard et al, 2008] communication. The ultimate limit for correcting errors from a given channel is called the capacity of the channel. While it is not yet known how to compute the capacity from a description of a given channel, we made an intriguing and counter-intuitive discovery [Smith & Yard, 2008]: by considering a pair of channels that each have zero capacitance if operating separately, we showed that they can allow noiseless communication when combined, see Fig. 5. This result reveals an unanticipated, rich structure in the theory of quantum communication which deepens the relationship between quantum cryptography and quantum coherence, while giving new hope for protecting quantum systems from noise which was previously thought to be detrimental.

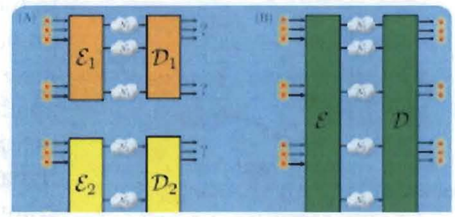
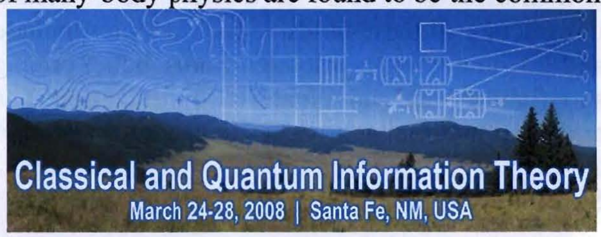


Fig. 5 Quantum channels are not additive 0+0 > 0!

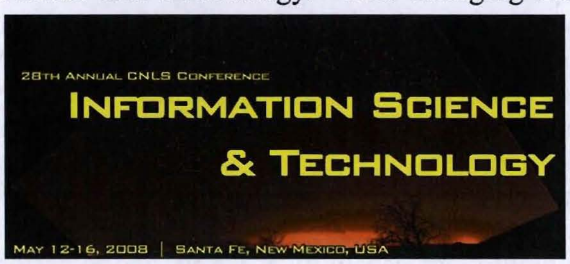
At the interface of quantum information and quantum physics lies an interesting set of fundamental problems in quantum mechanics. For example, in spite of the intense interest accorded to the Quantum Hall Effect in the past four decades, and in spite of spectacular breakthroughs, there is still no first-principles proof of the integer or fractional quantization for interacting electron systems. The current understanding is based on an argument that averages over a fictitious magnetic flux. Many proofs of the quantization of the Hall conductance involve a cyclic adiabatic evolution of the ground state under a slowly varying flux, which maps the original ground state to the same state up to what is known as a Berry phase. The averaging argument is then used to show that the Hall conductance corresponds to a Chern number and is thus an integer (or, a fraction in the case of ground state degeneracy). Using the technique of quasi-adiabatic evolution recently developed by a CNLS affiliate, CNLS researchers are attempting to show quantization of the Hall conductance up to exponentially small corrections in the size of the system, without the restriction of averaging. If successful, this would settle an important and fundamental open problem in mathematical physics.

Related Activities

The CNLS-sponsored conference Classical and Quantum Information Theory was held in March, 2008. Over half a century ago, it was realized that quantum and statistical field theories are intimately related, both at the formal and physical levels. Quantum critical phenomena provide examples where quantum systems are frequently mapped onto classical systems, whereas non-equilibrium statistical mechanics provides an example of proceeding in the other direction via stochastic operator techniques. We are now witnessing a similar phenomenon in the areas of classical and quantum information theory, where methods and concepts of many-body physics are found to be the common element for seemingly different problems such as quantum and classical spin glasses and quantum and classical error correcting codes. Our workshop explored these developments, inviting leading experts to discuss the latest problems and techniques of interest. We discussed various questions at the interface of these fields including possible new behaviors in quantum spin glasses due to entanglement and the role of message passing algorithms for quantum systems, both for decoding of error correcting codes and for finding ground and thermal states. This conference brought together experts from classical and quantum information theory, statistical physics and computer science, and both improved communication and contributed to a coherent description of this class of problems.



In May 2008, the CNLS sponsored the 28th CNLS Annual Conference "Information Science and Technology." This emerging Laboratory topic will be a cornerstone of scientific advances in the 21st century. New technologies will produce quantitative measurements in systems that could hitherto only be studied qualitatively. Further, the size of datasets in scientific, commercial, and government applications will continue to grow exponentially, in some cases reaching petabyte and exabyte scales. This shift from hypothesis-driven to data-driven science is creating opportunities to accelerate discoveries in science and technology and to apply these discoveries to problems of national and global importance. The 28th CNLS Annual Conference brought together experts from a variety of disciplines which impact information science and technology. Specific areas included information theory, machine learning, massive datasets, quantitative finance, bioinformatics, astroinformatics, statistics, neurocomputing, and image analysis.



In August, 2009, the CNLS will sponsor a new information science and technology related conference entitled "Physics of Algorithms." Optimization, inference and learning involve emerging computational problems in many areas of science and engineering. Typically stated in the framework of computer science and information theory, these problems are also linked to concepts and approaches native to statistical, mathematical and quantum physics. This interdisciplinary field has a seen a recent explosion of activity, resulting in new algorithms and new methods of analysis. Discrete computational challenges including constraint satisfaction and error correction have benefited from techniques and insights offered by statistical physics. Physics, at the same time, has been significantly enriched by approaches from discrete computation, such as convex optimization and message-passing algorithms. This conference brings together leading experts from physics, computer science, machine learning, operations research and information theory to discuss the current hot topics and new challenges at the intersection of these fields. Specific topics include graphical models, statistical inference and learning, monte carlo algorithms, belief propagation and message-passing algorithms, satisfiability and combinatorial optimization, phase transitions and cavity approaches, and combinatorial approaches relevant to random walks, loops, etc.

Summary

The work at CNLS in information science and technology, through scientific research in general approaches to IS&T as well as in applications of the approach in physical, chemical and biological systems has had important LANL impact. A major new thrust in IS&T is emerging in a number of Laboratory Divisions including T, CCS, HPC, D, and ISR. CNLS is playing a leading role in that development through its own scientific activities and in close collaboration with the new incubation Information Science and Technology Center. By nurturing new ideas, making surprising connections among disparate subjects in an interdisciplinary manner, and by bringing together fundamental science paired with applications, CNLS is playing a pivotal role in bringing this field into prominence at LANL. Of particular importance are the connections between statistical physics and the computer/information science of inference, new discoveries and connections between classical and quantum information, emerging efforts in cognitive neuroscience and computing, and the continuing utilization of network theory applied to a number of important problems. The range of publications reflects the diversity of our efforts, from *Science* and *Physical Review Letters* to *IEEE Transactions* and *Knowledge-Based Systems,* but a firm grounding in quantitative methods and physics background ties things together in a productive manner. We look forward to the next 18 months of this proposal as a continuing opportunity to build IS&T capability at LANL and to perform world-class science that enhances the interdisciplinary environment at CNLS.

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