

Resúmenes Conferencias Magistrales 4aRNCSCyST 2011

Data integration, systems approach and multilevel description of complex biosystems

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Recent years have witnessed the development of new quantitative approaches and theoretical tenets in the biological sciences. The advent of high throughput experiments in genomics, proteomics and electrophysiology (to cite just a few examples) have provided the researchers with unprecedented amounts of data to be analyzed. Large datasets, however can not provide the means to achieve a complete understanding of the underlying biological phenomena, unless they are supplied with a solid theoretical framework and with proper analytical tools.

It is now widely accepted that by using and extending some of the paradigmatic principles of what has been called 'complex systems theory', some degree of advance in this direction can be attained. In this talk I will be presenting ways in which by using data integration techniques (linear, non-linear, combinatorial, graphical), multidimensional-multilevel descriptions (multifractal modeling, dimensionality reduction, computational learning), as well as an approach based in systems theory (interaction maps, probabilistic graphical models, non-equilibrium physics) have allowed us to better understand some problems in the interface of Statistical Physics and Computational Biology.

Counting and Classifying

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The theme of this talk is the allocation of n objects (or elements) into g categories (or classes), discussed from several viewpoints. This approach can be traced back to the early work of 24-year-old Ludwig Boltzmann in his first attempt to derive Maxwell's distribution of velocity for a perfect gas in probabilistic terms. I will briefly explain how to describe the state of affairs in which for every object listed 'alphabetically' or in a sampling order, its category is given. We can consider these descriptions as facts (taking place or not), and events as propositions (true or not) about facts (taking place or not). Not everything in the world is known, and what remains is a set of possibilities. For this reason, I show how events can be probabilized and rephrased in the powerful language of random variables and stochastic processes. Even if the problem of allocating n objects into g categories may seem trivial, it turns out that many important problems in statistical physics and some problems in economics and finance can be formulated and solved using the methods described.

Equilibrium and nonequilibrium properties of economic exchange models

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Economic exchange, e.g. through commerce, has been an important factor in shaping human societies, even driving their development according to some. However, to date there is no consensus as to which (simple) mathematical model better captures the most important properties of economic exchange. Several possibilities will be discussed and analyzed, stressing the relevance of two essential ingredients: multiplicativity and randomness. It is shown that these two can, together, give rise to counterintuitive economic phenomena.

Synergy Between Biology and Mathematics: Past, Present and Future

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Although biology and mathematics have long been intertwined over the last half millennium, an explosive synergy between biology and mathematics seem poised to enrich and extend both fields and biomedical engineering greatly in the coming decades. The avalanche of biological data generated by contemporary high-throughput computational biology has changed the traditional landscape of biology. As a science, biology depends increasingly on data, algorithms, and models in virtually every respect. It is becoming more quantitative, more computational, and more mathematical. All three methods-quantitative, computational, mathematical-are spreading across the entire landscape of biological science, from molecular to cellular, organismic, and ecological. Two disciplines that have extraordinary potential to meet these biological challenges are mathematics, computer science, and bioinformatics. The outline of this talk includes three phases of the synergy between biology and mathematics:

Part 1 The Past

- The Motion of the Heart and Blood in Animals (Harvey 1847)
- Discovery of Genes (Mendel 1866)
- Biological Problems that Stimulated Mathematics
- Ten Equations that Changed Biology

Part 2 The Present

- The Landscapes of Biological Sciences
- The Landscapes of Applied Mathematics
- The Landscapes of Research in Biology and Mathematics
- Bioinformatics of Mathematics: Theory, Methods, and Applications

Part 3 The Future

- Potential Problems
- Meeting the Challenges: Education Across the Biological, Mathematical and Computer Sciences
- A New Biology Curriculum for the 21st Century
- Ten Challenges in the Synergy Between Biology and Mathematics

Simulation Protein Evolution and Higher Order Amino Acid-Substitution Groups with an Empirical Codon-Substitution Matrix.

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Background: Understanding protein evolution remains a major challenge in molecular biology. Considering only point mutations, it involves at least four abstract spaces: 1) A genotype space, where codon mutations occur; 2) a protein-sequence space, where the corresponding amino acid changes take place, according to the rules dictated by the genetic code; 3) a protein-structure space, where the changes are evaluated in physical-chemical terms; and, 4) a phenotype space, where natural selection operates. Here, we are interested in commonly allowed single-base codon mutations corresponding to amino acid substitutions which obey general physical chemical constraints that determine overall conservation.

Results: To determine the general nature of the mutations that can be accepted by orthologous proteins, we simulate the divergence process in proteins that maintain the same or very similar functions and structures. For this simulation, we employed an empirically derived Markov model of codon substitution that is provided in the literature. We found that about 83% of most frequent amino acid substitutions generated in our simulations agree with the empirically found substitutions, coming from three data sets, reported by Sasidharan and Choithia (The selection of acceptable protein mutations. PNAS, June 12, 2007; vol. 104, no.24. pp 10080–10085). It is well known that, from the nature of genetic code and underlying biases, codons tend to cluster into almost invariant sets having a high rate of changes among codons of each set but very small rates between sets. These sets define higher order amino acid-substitution groups (reduced alphabets). The groups we obtained in our simulations agree with the higher order dynamics on the level of amino acid groups, obtained theoretically from the same empirical codon substitution matrix by Görnerup and Jacobi (BMC Bioinformatics 2010, 11:201).

Conclusions: In molecular evolution, the substitution process hierarchically operates on multiple levels, from nucleotides to codons to groups of codons. As remarked by Görnerup and Jacobi, each level approximately has its own closed dynamics. The original dynamics and the partition of the state space then define a new stochastic process on the coarser level. These theoretic aspects of evolution seem to be corroborated by our simulations.

Thermodynamics & Complexity

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A link between entropy and information is established. It is discussed the incompatibility between the macroscopic irreversibility and microscopic reversibility, also the entropy production principle and its different and sometimes contradictory statements. The entropy production rate is properly related to aging and cancer.

Life, Solar Photon Dissipation, and the Water Cycle

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Since its inception some 3.8 billion years ago, life has been intimately connected with the hydrological cycle. Through various physical-chemical mechanisms, life has conserved the amount of water on Earth, has kept Earth's temperature within the narrow range suitable for the three phases of water, and has augmented the amount of water in the water cycle. This biotic-

abiotic coupling is argued to be a manifestation of established non-equilibrium thermodynamic principles which indicate that irreversible processes couple to remove impediments to greater global entropy production. Biology, dispersed throughout Earth's surface, has adjusted the gases of Earth's atmosphere in such a manner that the most intense part of the solar spectrum can penetrate the atmosphere and reach the surface to be intercepted by biology. The covalent bonding of atoms in organic pigments leads to collective electronic excitations compatible with these high photon energies. Inter-system crossing and vibrational relaxation to the ground state of these excited molecules when in water leads to rapid dissipation of the solar photons into heat, and this is the major source of entropy production on Earth. An important part of the energy of the dissipated photons is channeled into the hydrological cycle through the latent heat of vaporization of surface water. By dissipating the ensuing surface to atmosphere temperature gradient, the hydrological cycle further increases the entropy production of Earth. This thermodynamic view has implications to the origin of life, a more general theory of evolution, and to the theory of Gaia.

El atractor de una red de mapeos contractivos acoplados

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Las redes de mapeos contractivos han sido usadas para modelar la dinámica de algunas redes biológicas como las redes de regulación genética y las redes neuronales. Presentaré algunos resultados generales sobre la estructura topológica del atractor de estas redes, algunos ejemplos "anómalos" y algunas conjeturas sobre el comportamiento esperado en el caso regular.

Non-elastic billiard models

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In billiard models, a point particle collides with a fixed boundary. When the collision is elastic (specular), this gives rise to a Hamiltonian dynamics which can exhibit different phenomena, including integrability, (Hamiltonian) chaos, and mixed dynamics, depending on the shape of the boundary. In this talk, we will discuss results on the effect of changing the collision rule so that the dynamics becomes dissipative. In this case, we observe a range of behaviour, including attracting periodic orbits and chaotic strange attractors. We will focus on recent work on non-elastic polygonal billiards, joint with Aubin Arroyo and Roberto Markarian, in which these phenomena can be explored in more detail.

Flujos súper acelerados

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Presentamos un estudio teórico del flujo súper acelerado generado por un líquido inviscido contenido en un tubo cónico vertical y en dos tubos interconectados de diferente radio cuando el fondo de ambos es abierto súbitamente. En ambos casos analizamos el comportamiento de la superficie libre, las inestabilidades de ésta y la transformación de la energía potencial en energía cinética.

Complejidad y propiedades físicas de fluidos magneto-reológicos

José Luis Carrillo Estrada

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La estructura que forman las partículas al agregarse en una dispersión magneto-reológica, cuando es expuesta a un campo magnético estático, tiene características multifractales. Si además del campo estático estas dispersiones se exponen a una perturbación magnética, la estructura muestra una complejidad evolutiva, que es acompañada por cambios muy importantes en las propiedades físicas del sistema. A bajas concentraciones de partículas, los patrones de estructura son drásticamente diferentes, pero aún una perturbación magnética produce cambios espectaculares en las propiedades físicas de la dispersión. Se discuten a este respecto resultados experimentales y modelos que permiten entender la razón física de los cambios producidos por las perturbaciones.

Curso: Introducción a los sistemas dinámicos

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