Entropy 2018 – From Physics to Information Sciences and Geometry

Faculty of Biology

University of Barcelona

Barcelona, Spain

14 – 16 May 2018

Conference Chair

Prof. Dr. Ali Mohammad-Djafari

Conference Co-Chair

Prof. Dr. Miguel Rubi

Organised by

MDPI

Conference Secretariat

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#Entropy2018

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Entropy 2018 – From Physics to Information Sciences and Geometry

14 – 16 May 2018, Barcelona, Spain

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	Coffee Break & Poster Session (S1, S2 & S3)	**Coffee Break & Poster Session (S1, S2 & S3)**	**Coffee Break & Poster Session (S4, S5 & S6)**
	Session 1. Part B	*Session 3. Part B*	*Session 6. Part A*
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Afternoon	*Session 2*	*Session 4. Part A*	*Session 6. Part B*
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Monday 14 May 2018: 08:00 - 12:45 / 14:15 - 18:00

Tuesday 15 May 2018: 08:30 - 12:30 / 14:00 - 18:00 / Conference Dinner: 20.30

Wednesday 16 May 2018: 08:30 - 12:15 / 13:45 - 18:00

Conference Programme

Monday 14 May 2018

08:00	Registration Desk Open (Check-in)
08:45 – 09:00	Opening Ceremony Chairs: Ali Mohammad-Djafari and Miguel Rubi

Session 1
Physics: Classical Thermodynamics and Quantum
Part A
Chairs: Ariel Caticha and Dick Bedeaux

09:00 – 09:30	**Dick Bedeaux** "Non-Isothermal Transport of Immiscible Fluids in a Porous Material: Surface and Line Contributions to Driving Forces"
09:30 – 09:45	**Mark Masthay** "Eigenstate-Specific Temperatures in Two-Level Systems: Potential Applications to Nanothermometry and the Negative Temperature Debate"
09:45 – 10:00	**José Ortiz De Zarate** "Casimir Effects on Giant Fluctuations"
10:00 – 10:15	**Eugenio Vogel** "Thermodynamics of Magnetism for Particles with Small Number of Elements"
10:15 – 10:30	**Andrés Santos** "Residual Multiparticle Entropy for a Fractal Fluid of Hard Spheres"
10:30 – 11:15	**Coffee Break & Poster Session (S1, S2 & S3)** Chair: **Miguel Rubi**

Session 1. Part B
Physics: Information and Quantum Geometry
Chairs: Dick Bedeaux and Ariel Caticha

11:15 – 11:45	**Ariel Caticha** "From Information Geometry to Quantum Geometry"
11:45 – 12:00	**Liliana Luca** "Comparing Linear and Nonlinear Hydrodynamical Models for Charge Transport in Graphene Based on the Maximum Entropy Principle"
12:00 – 12:15	**Ralf Eichhorn** "Active Forcing as a Non-Equilibrium Environment for Brownian Motion: Fluctuation Theorem and Mutual Information"

12:15 – 12:30	**Rodrigo de Miguel** "Temperature-Dependent Spectra and the Thermodynamics of Small Systems"
12:30 – 12:45	**Nicolai Friis** "Gaussian Operations for Work Extraction and Storage" - Entropy 2018 Young Investigator Award Winner
12:45 – 14:15	**Lunch**

Session 2
Statistical Physics and Bayesian Computation

Chairs: Ercan Kuruoglu and Jean-Christophe Pesquet

14:15 – 14:45	**David Wolpert** "Fundamental Limits on the Thermodynamics of Circuits"
14:45 – 15:00	**Karl Heinz Hoffmann** "The Entropy Production Paradox for Fractional Diffusion"
15:00 – 15:15	**Sergio Davis** "Emergence of Tsallis Statistics as a Consequence of Invariance"
15:15 – 15:30	**Natalya Denisova** "Bayesian Approach with Local Regularization for Solving Reconstruction Problems"
15:30 – 15:45	**Ricardo T. Páez-Hernández** "The Entropy of a Classical Ideal Gas Whose Distribution Speed Law Is a Stretched Exponential Function"
15:45 – 16:30	**Coffee Break & Poster Session (S1, S2 & S3)** Chair: **Kevin Knuth**

Special Session
Fourier 250th Birthday: Geometric Theory of Thermodynamics

Chairs: Fréderic Barbaresco and Ali Mohammad-Djafari

16:30 – 16:45	**François Gay-Balmaz** "A Variational Formulation for the Non-Equilibrium Thermodynamics of Open Systems"
16:45 – 17:00	**Hiroaki Yoshimura** "Dirac Structures, Interconnections, and Variational Formulations in Non-Equilibrium Thermodynamics"
17:00 – 17:15	**José Isidro** "On the Contact Geometry and the Poisson Geometry of the Ideal Gas"
17:15 – 17:30	**Luisberis Velazquez Abad** "Riemannian Geometry of Fluctuation Theory: A Counterpart Approach of Information Geometry"
17:30 – 18:00	**Frédéric Barbaresco** "Geometric Theory of Information and Heat Based on Souriau Lie Groups Thermodynamics for Machine Learning"

Tuesday 15 May 2018

Session 3
Geometrical Science of Information, Topology and Metrics
Part A
Entropy, Information Geometry and Quantum States
Chairs: Jun Zhang and Pierre Baudot

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09:00 – 09:30	**Nina Amini** "Non-Linear Filtering and Entropy Production"
09:30 – 09:45	**Jan Naudts** "Challenges in Non-Commutative Information Geometry"
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10:00 – 10:15	**Eun-jin Kim** "Information Geometry in Classical and Quantum Systems"
10:15 – 10:30	**Rainer Hollerbach** "Far-From-Equilibrium Time Evolution between Two Gamma Distributions"
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Session 3. Part B
Entropy, Information Geometry, Topology and Metrics
Chairs: Ali Tahzibi and Nina Amini

11:00 – 11:30	**Pierre Baudot** "Topological Information Data Analysis: Statistical Physic of Complex Systems, Application to Genetic Landscapes"
11:30 – 12:00	**Stefano Mancini** "Hamilton-Jacobi Approach to Potential Functions in Information Geometry"
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Session 4
Maximum Entropy Principle and Inference
Part A

Chairs: Ali Mohammad-Djafari and Jean-François Bercher

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14:30 – 15:00	**Robert Niven** "Maximum Entropy Analysis of Electrical, Water and Transport Networks"
15:00 – 15:15	**Jun Zhang** "Information Geometry Under Monotone Embedding"
15:15 – 15:30	**William Bruce Sherwin** "Entropy Unifies Ecology and Evolution"
15:30 – 16:00	**Coffee Break & Poster Session (S4, S5 & S6)** Chairs: **Stefano Mancini**

Session 4. Part B

Entropy, Information, Topology and Metrics

Chairs: Adom Giffin and Robert Niven

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16:30 – 17:00	**Kevin Knuth** "Entropy and Relevance among Questions"
17:00 – 17:30	**Ercan Kuruoglu** "In Search of the Optimal Genetic Code: 'What Does the Information Theory Have to Say about Evolution?"
17:30 – 17:45	**Jan Korbel** "Consistency of the Maximum Entropy Principle for Generalized Entropies"
17:45 – 18:00	**Stephan Weis** "A New Signature of Quantum Phase Transitions from the Numerical Range"
18:00	Conference Group Photograph
20:30	**Conference Dinner**

Wednesday 16 May 2018

Session 5
Kullback and Bayes or Information Theory and Bayesian Inference

Chairs: Stefano Mancini and Pierre Baudot

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09:00 – 09:15	**Peishi Jiang** "Interactions of Information Transfer Along Separable Causal Paths"
09:15 – 09:30	**Badr Albanna** "How Much Information Is Shared by Three Variables? Principled Generalizations of the Mutual Information to Three or More Variables"
09:30 – 09:45	**Frank Lad** "The Duality of Extropy/Entropy, and the Completion of the Kullback Information Complex"
09:45 – 10:00	**Jakob Knollmüller** "Separating Diffuse from Point-Like Sources - a Bayesian Approach"
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Session 6
Entropy in Action (Applications)

Part A

Chair: Ali Mohammad-Djafari

10:45 – 11:15	**Jose M. G. Vilar** "Biophysical and Biomedical Applications of the Gibbs Entropy Postulate"
11:15 – 11:45	**Olivier Rioul** "On Minimum Entropy and Gaussian Transport"
11:45 – 12:00	**Allison Goodwell** "Temporal Information Partitioning Networks Reveal Ecohydrologic Responses to Rainfall Pulses and Drought"
12:00 – 12:15	**Gordon Morison** "Multiscale Weighted Permutation Entropy Analysis of the EEG in Early Stage Alzheimer Patients"
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Session 6. Part B

Chair: Ali Mohammad-Djafari and Paul Baggenstoss

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14:15 – 14:45	**Mohammad Modarres** "Entropy as an Indicator of Damage in Engineering Materials"
14:45 – 15:00	**Marios Valavanides** "Estimation of the Number Density of Configurational Microstates in Steady-State Two-Phase Flows in Model Porous Media"
15:00 – 15:15	**Ishay Wohl** "Fluctuation of Information Entropy Measures in Cell Image"
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Session 6. Part C

Chairs: David Reguera and Mohammad Modarres

16:00 – 16:30	**Paul Baggenstoss** "Maximum Entropy PDF Projection: Applications in Machine Learning"
16:30 – 16:45	**Carlos Granero-Belinchon** "A Kullback-Leibler Divergence Measure of Intermittency: Application to Turbulence"
16:45 – 17:00	**Karsten Keller** "Change-Point Detection Using the Conditional Entropy of Ordinal Patterns"
17:00 – 17:15	**Simon Schultz** "Dynamical Entropy Measures to Diagnose Deficits in Mouse Spatial Exploration Behaviour"
17:15 – 17:30	**Martin Goethe** "Prediction of Protein Configurational Entropy (Popcoen)"
17:30 – 17:45	**Alain Le Bot** "Entropy in Statistical Sound and Vibration: from Macroscopic to Super-Macroscopic World"
17:45 – 18:00	**Closing Remarks and Awards Ceremony**

Welcome by A. Mohammad-Djafari and Miguel Rubi

Dear Colleagues,

It is with great pleasure that we welcome you to the conference "Entropy 2018: From Physics to Information Sciences and Geometry" organized and sponsored by the MDPI open-access journal *Entropy*, in Barcelona. We would like to thank you for the great response and interest on attending this event.

One of the most frequently used scientific words, is the word "Entropy". The reason is that it is related to two main scientific domains: physics and information theory. The origin of this word in physics is related to thermodynamics and the state of a system (Clausius, Carnot) and the relation between the macroscopic and microscopic states in statistical physics (Boltzmann, Gibs, Maxwell) and in Quantum mechanics by Von Neumann. Its origin in Information theory goes back to Shannon. Since those origins, many definitions and extensions have been proposed and used. We may mention here only a very few of them: Gibbs entropy: the statistical mechanical entropy of a thermodynamic system; Boltzmann entropy: Gibbs entropy when neglecting internal statistical correlations in the overall particle distribution; Shannon Information entropy: the average amount of information produced by a stochastic source of data; Tsallis entropy: a generalization of the Boltzmann–Gibbs entropy; Rényi entropy: a generalization of Shannon entropy. We may also mention the Maximum Entropy Principle of Jaynes and its extensions via the Cross Entropy or Relative entropy (Kullback-Leibler).

This conference is an opportunity to bring international researchers from these communities together and create synergies, not only from theoretical perspectives, but also from a practical point of view and applications.

During this exciting three-day conference, you will be able to enjoy the newest researches on the field, through different talks and discussions in a comfortable, relaxed and academic environment.

We hope that you all have a great experience and enjoy your stay in Barcelona!

Ali Mohammad-Djafari
Conference Chair

CNRS, L2S, CentraleSupélec,
University Paris Saclay, France

Miguel Rubi
Local Chair

Department of Condensed Matter
Physics at the University of
Barcelona, Spain

Entropy (ISSN 1099-4300; CODEN: ENTRFG) is an international and interdisciplinary open access journal of entropy and information studies, published monthly online by MDPI. *Entropy* deals with the development and/or application of entropy or information-theoretic concepts in a wide variety of applications. Relevant submissions ought to focus on (i) developing the theory behind entropy or information theory, (ii) providing new insights into entropy or information-theoretic concepts, (iii) demonstrating a novel use of entropy or information-theoretic concepts in an application, or (iv) obtaining new results using concepts of entropy or information theory.

Among other databases, *Entropy* is indexed by the Science Citation Index Expanded (Web of Science) MathSciNet (AMS), Inspec (IET), and Scopus.

Journal Webpage: http://www.mdpi.com/journal/entropy
Impact factor: 1.821 (2016); 5-Year Impact Factor: 1.947 (2016)

General Information

MDPI, the Multidisciplinary Digital Publishing Institute, is an academic open access publisher, established in 1996. We publish over 180 peer-reviewed open access journals across ten different subject areas and offer publishing-related initiatives to scholars:

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If you would like more information about open access or any of our services listed above, be sure to talk to us at the conference. See you there!

Entropy 2018 – From Physics to Information Sciences and Geometry will be held at the Faculty of Biology, University of Barcelona, on 14 – 16 May 2018.

This conference is an opportunity to bring international researchers from these communities together and create synergies, not only from theoretical perspectives, but also from a practical point of view and applications. During this exciting three-day conference, you will be able to enjoy the newest researches on the field, through different talks and discussions in a comfortable, relaxed and academic environment.

Conference Venue

Faculty of Biology, University of Barcelona
Avinguda Diagonal, 643, 08028 Barcelona, Spain

Registration Desk

The desk for registration, information and distribution of documents will be open from 08:00 on 14 May 2018.

Certificate of Attendance

Upon request, the participants of the event will receive an electronic Certificate of Attendance by email once the event is concluded.

Barcelona and Catalonia

Catalonia has become one of the favourite tourist destinations of Spain, mainly because of Barcelona, a city that never sleeps and knows how to please the big majority. With a history among the oldest in Europe, Barcelona offers a mixture of inland and seaside charms that panders the interests of everybody. The variety of artistic treasures, Romanesque churches and the works of famous artists such as Dalí, Gaudí, Miró or Picasso will make of your visit to the city a remarkable experience.

Barcelona is the capital and largest city of Catalonia and Spain’s second largest city, with a population of over one and half million people (over five million in the whole province).

This city, bathed by the Mediterranean Sea, has become one of most cosmopolitan cities of Europe which has transformed it into the very modern, yet incredibly old city.

This beautiful city is full of what European cities are known for (outdoor markets, restaurants, shops, museums and churches) and which makes it the perfect scenario to get lost in its picturesque streets and avenues. Moreover, Barcelona’s extensive and reliable Metro system will take you to more far-flung destinations. The core centre of the town, focused around the *Ciutat Vella* ("Old City"), provides days of enjoyment for those looking to experience the life of Barcelona while the beaches the city was built upon provide sun and relaxation during the long periods of agreeably warm weather. [Source: www.wikitravel.org].

Plaza Espanya (Source: www.viajero-turismo.com)

The Faculty of Biology, University of Barcelona

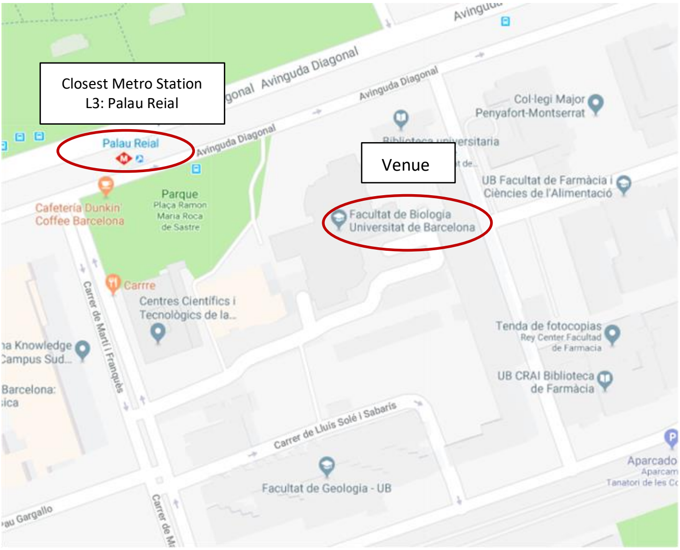
The conference will be held at the Faculty of Biology of the University of Barcelona. Established in 1974, it became a pioneering institution in Spain and first appeared as a result of increasing knowledge in the field of life sciences at a time of relentless diversification.

The University of Barcelona (UB) is the most formidable public institution of higher education in Catalonia, catering to the needs of the greatest number of students and delivering the broadest and most comprehensive offering in higher educational courses. The UB is also the principal centre of university research in Spain and has become a European benchmark for research activity, both in terms of the number of research programmes it conducts and the excellence these have achieved.

Having been founded in 1450, the University's own history is closely tied to the history of Barcelona and Catalonia, it combines the values of tradition with its position as an institution dedicated to innovation and teaching excellence: a university that is as outward-looking and cosmopolitan as the city from which it takes its name. For these reasons, it plays a direct and active part in the urban fabric of Barcelona, becoming a hub of cultural activity for the city itself. [Source: www.ub.edu].

How to Reach the Venue

Address: Avinguda Diagonal, 643, 08028 Barcelona, Spain



Venue Location (Source: www.google.es/maps/)

Conference Dinner

Tuesday 15 May, 20:30

The conference dinner will be held at Marina Bay, a cutting-edge restaurant specialised in Mediterranean cuisine which, in addition to its location in front of the Port Olympic of Barcelona, will make of your evening at the restaurant an experience to remember.

Marina Bay is located at Calle de la Marina, 19-21, only a few minutes away from one of one of Barcelona's most emblematic must-sees, the famous Frank Gehry "Golden Fish" statue. You can easily reach the restaurant from the conference venue either by taxi or by Metro. If you were to choose the second option, the closest metro station is "Ciutadella/Vila Olimpica" on Line 4 (from the conference Venue, you can take the metro Line 3 at Palau Reial station, and change to Line 4 at Passeig de Gràcia station).

Contact persons during the event

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Emergency Information

All emergencies in Spain: 112 (no area code needed)

Ambulance (Ambulancia) and health emergencies: 061 or 112
Fire brigade (Cuerpo de bomberos): 080 or 112
Spanish National Police (Policía nacional): 091

Abstracts

Session 1. Physics: Classical Thermodynamics and Quantum

Non-Isothermal Transport of Immiscible Fluids in a Porous Material: Surface and Line Contributions to Driving Forces

Dick Bedeaux, Signe Kjelstrup

Department of Chemistry, PoreLab, Trondheim, Norway

We derive the entropy production for the transport of heat and two immiscible fluids in an inelastic porous material. The representative volume elements (REVs) are described by their entropy, energy, volume and masses. The Gibbs equation defines their temperature, pressure and chemical potentials.

Constitutive equations that follow from the entropy production of the REVs can be written for a continuous path in state space. There are three independent driving forces and conjugate fluxes, one for the transport of heat and two for the transport of two immiscible fluids. The forces contain contributions from surface and line energies, contributions that are important at low capillary numbers.

The equations predict a Soret effect and can be used to compute thermal osmosis. They provide an explanation for observations that have been known for a long time, i.e., that there are deviations from Darcy's law at low capillary numbers [1–4] for transport in clay soil even through glass beads. We find out how volume flow arises, not only from changes in the pressure, but also from changes in the porosity, or saturation of the wetting fluid, temperature and chemical potentials. We discuss how the relations can be tested by non-equilibrium molecular dynamics simulations or experiments.

References:

1. Miller, R.J.; Low, P.F. Threshold Gradient for Water Flow in Clay Systems. *Soil Sci. Soc. Am. Proc.* **1963**, *27*, 605–609.
2. Swartzendruber, D. Non-Darcy Flow Behaviour in Liquid-Saturated Porous Media. *J. Geophys. Res.* **1962**, *67*, 5205–5213.
3. Bernandiner, M.G.; Protopapas, A.L. Progress on the Theory of Flow in Geologic Media with Threshold Gradient. *J. Environ. Sci. Health* **1994**, *A29*, 249–275.
4. Boersma, L.; Lindström, F.T.; Saxena, S.K. Limitations of Darcy's law in glass bead porous media. *Soil Sci. Soc. Am. Proc.* **1973**, *37*, 333–335

NOTES

Eigenstate-Specific Temperatures in Two-Level Systems: Potential Applications to Nanothermometry and the Negative Temperature Debate

Mark Masthay [1], Robert Gerald Keil [1], Calley N. Eads [2], Amber N. Johnson [1], Joe D. Mashburn [3], Harry B. Fannin [4]

[1] *Department of Chemistry, The University of Dayton, Dayton, OH, USA*
[2] *Department of Chemistry and Biochemistry, The University of Arizona, Tuscon, AZ, USA*
[3] *Department of Mathematics, University of Dayton, Dayton, OH, USA*
[4] *Department of Chemistry, Murray State University, Murray, KY, USA*

Four eigenstate-specific temperatures (ESTs) have been derived for two-level paramagnetic spin lattices (see *J. Chem. Phys.* 147, 214306 [2017]). Microcanonical and canonical “Boltzmann” ESTs, defined as derivatives $(dU/dS)_V$, are designated “continuous”; microcanonical and canonical ESTs, defined as finite difference ratios (delta$U$/delta$S$)$_V$, are designated “discrete”. They are calculated using microcanonical ($S_{Bu}[U_j] = k$ ln$[N!/(N - j)!j!]$ and canonical ($S_{Bc}[U_j] = k$ ln $N^N/[N - j]^{[N-j]}j^j$) *Boltzmann* entropies. Reported comparisons of T_c to T_{du} potentially confound the relative impacts of condition (microcanonical or canonical) and smoothness (continuous or discrete) on temperature. The four ESTs allow for direct comparisons of T_u to T_c, T_{du} to T_{dc}, T_u to T_{du}, and T_c to T_{dc}—thus minimizing these potential ambiguities. At large N, the four ESTs are intensive, equal to the bath temperature T_c^{bath}, and obey all four laws of thermodynamics; for N 1000, the ESTs are generally non-intensive, not equal to T_c^{bath}, and violate the four laws. Nevertheless, each EST manifests an energy dependence which quantifies its deviation from T_c^{bath}. The ESTs are thus good *temperature estimators* at small N, making them potentially useful in nanothermometry. The four “Boltzmann” ESTs detailed above are positive for eigenstates below the energy median, but negative for population-inverted eigenstates. In contrast, their “Gibbs” EST counterparts—calculated with microcanonical ($S_{Gu}[Uj]$) and canonical ($S_{Gc}[U_j]$) *Gibbs* entropies—are uniformly positive. The relative merits of “Boltzmann” and “Gibbs” ESTs will be detailed in light of the ongoing negative temperature debate.

NOTES

Casimir Effects on Giant Fluctuations

Jose Ortiz de Zarate

Complutense University of Madrid, Madrid, Spain

In my presentation, I shall review work performed in the last two decades, which extended Landau–Lifshitz Fluctuating Hydrodynamics for the evaluation of spontaneous thermal fluctuations around non-equilibrium (NEFs) steady states [1]. This work relies on the adoption of a local equilibrium version of the fluctuation–dissipation theorem for dissipative fluxes. It turns out that mode-coupling phenomena that do not exist in equilibrium, cause, in many instances, the NEFs to be strongly enhanced. Moreover, opposite to equilibrium ones, equal-time NEFs have, generically, a long spatial range, not limited to the close vicinity of (equilibrium) critical points. The combination of these two characteristics leads these NEFs to be referred to as **Giant Fluctuations**. In addition, the generic long-spatial-range causes the presence of boundaries (walls) to strongly affect the NEFs' spatio-temporal spectrum, including the recently predicted appearance of NEFS-induced **Casimir forces** [2]. I shall also briefly present the past experimental confirmation of several features of NEFs, as well as planned future space experiments [3] in which I participate. The strong experimental evidence leads one to conclude that any proposed thermodynamic potential (including entropy) for systems that are not in equilibrium has to be consistent with Fluctuating Hydrodynamics. In particular, most likely implying non-locality in space.

References:
1. de Zárate, J.M.O.; Sengers, J.V. *Hydrodynamic Fluctuations in Fluids and Fluid Mixtures*; Elsevier: Amsterdam, The Netherlands, 2006.
2. Kirkpatrick, T.R.; de Zárate, J.M.O.; Sengers, J.V. Giant Casimir effect in fluids in nonequilibrium steady states. *Phys. Rev. Lett.* **2013**, *110*, 235902.
3. Baaske, P.; Bataller, H.; Braibanti, M.; Carpineti, M.; Cerbino, R.; Croccolo, F.; Donev, A.; Köhler, W.; Ortiz de Zárate, J.M.; Vailati, A. The NEUF-DIX space project. Non-EquilibriUm Fluctuations during DIffusion in compleX liquids. *Eur. Phys. J. E* **2016**, *39*, 119.

NOTES

Thermodynamics of Magnetism for Particles with a Small Number of Elements

Eugenio Vogel [1], Julio Valdés [1], Gonzalo Saravia [1], Patricio Vargas [2], Antonio José Ramirez-Pastor [3], Paulo Centres [3]

[1] *Department of Physics, University of La Frontera, Temuco, Chile*
[2] *Department of Physics, Universidad Santa Maria, Valparaíso, Chile*
[3] *National University of San Luis, San Luis, Argentina*

The statistical mechanical treatment of magnetism is examined using the well-known Ising and Potts (clock) models for the case of very small systems. Since the main laws of thermodynamics and statistical physics were derived for vary large systems in what is usually called the thermodynamic limit (TL), several questions arise when these concepts are used for particles with under one thousand elements (magnetic centers in our case). However, present technology allows us to deal with these molecular or subnanoscopic systems [1] where some of the assumptions valid in the TL are not valid in the usual way [2]. Computer simulations for simple examples based on the Ising and the clock models are carried out. We review the concepts of ergodic separation, magnetization reversal, average magnetization, critical temperature and others as the systems become very small. We identify features that need special care for systems with few magnetic centers. The results are discussed by means of two examples, namely, two magnetic sensors with two different purposes [3].

References:
1. Roy, R.; Hohng, S.; Ha, T. A practical guide to single-molecule FRET. *Nat. Methods* **2008**, *5*, 507.
2. Gross, D.H.E. *Microcanonical Thermodynamics: Phase Transitions in Small Systems*; World Scientific: Singapore, 2001.
3. Vogel, E.E.; Vargas, P.; Saravia, G.; Valdes, J.; Ramirez-Pastor, A.J.; Centres, P.M. Thermodynamics of Small Magnetic Particles. *Entropy* **2017**, *19*, 499.

NOTES

Residual Multiparticle Entropy for a Fractal Fluid of Hard Spheres

Andrés Santos [1], Franz Saija [2], Paolo Vittorio Giaquinta [3]

1 Department of Physics, University of Extremadura, Badajoz, Spain
[2] CNR-IPCF, Messina, Italy
[3] Department of Mathematics and Computer Science, Physics and Earth Sciences, University of Messina, Messina, Italy

The residual multiparticle entropy (RMPE) of a fluid [1] is defined as the difference between the excess entropy per particle (relative to an ideal gas with the same temperature and density), s_{ex}, and the pair-correlation contribution s_2. Thus, the RMPE represents the net contribution to s_{ex} due to spatial correlations involving three, four, or more particles. A heuristic criterion for freezing in two and three dimensions states that the RMPE vanishes for the fluid at the liquid–solid transition [1]. While the criterion seems to be less reliable in four and, especially, five dimensions [2,3], knowledge of the RMPE is important to assess the impact of non-pair multiparticle correlations on the entropy of the fluid, regardless of its usefulness as a freezing criterion.

Recently, an accurate and simple proposal for the thermodynamic and structural properties of a hard-sphere fluid in fractional dimension 1d3 [4] has been proposed [5]. The aim of this work is to use this approach to evaluate the RMPE as a function of both d and density. It is observed that, for any given dimensionality d, the RMPE takes negative values for small densities, reaches a negative minimum $\mathrm{RMPE}_{\mathrm{min}}$, and then rapidly increases, becoming positive beyond a certain density. Interestingly, while the packing fraction corresponding to $\mathrm{RMPE}_{\mathrm{min}}$ monotonically decreases as dimensionality increases, the value of the minimum itself exhibits a nonmonotonic behavior, reaching an absolute minimum at a fractional dimensionality $d = 2.35$.

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NOTES

From Information Geometry to Quantum Geometry

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Entropic Dynamics (ED) is a framework in which dynamical laws are derived as an application of entropic methods of inference. The central object is a probability distribution. Its dynamics is driven by entropy subject to constraints that are eventually codified into the phase of the wave function. The central concern is to identify the relevant physical constraints and, in particular, to specify how those constraints are updated.

In this talk, I describe how the information geometry of the space of probabilities is extended to the ensemble-phase space of probabilities and phases. The result is a highly symmetric Riemannian geometry that incorporates a symplectic and a complex structure. The Entropic Dynamics that preserves these structures is a Hamiltonian flow and the simplest Hamiltonian suggested by the extended metric leads to Quantum Mechanics. Thus, a dynamics that is driven by entropy and that reflects the underlying information geometry provides the reason for Hamiltonians and for complex numbers in quantum mechanics.

NOTES

Comparing Linear and Nonlinear Hydrodynamical Models for Charge Transport in Graphene Based on the Maximum Entropy Principle

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Recent years have witnessed increasing interest in 2D-materials due to their promising applications. The most investigated 2D-material is graphene which is considered as a potential new semiconductor material for future applications in nano-electronic and optoelectronic devices. The aim of this work is to simulate suspended monolayer graphene. A physically accurate model for charge transport is given by a semiclassical Boltzmann equation. Numerical solutions of the transport equation can be obtained, for example, via Direct Monte Carlo Simulation (DSMC) or by finite difference schemes or by discontinuous Galerkin (DG) methods. However, these simulations have been obtained for simple cases such as in pristine graphene under an external constant electric field. With a view to more complex situations, it is desirable to benefit from simpler models such as drift-diffusion, energy transport or hydrodynamical ones. These directly provide balance equations for macroscopic quantities such as electron density, average velocity or current, average energy, etc., and, therefore, are more suited as models for CAD tools. In this work, two hydrodynamical models for charge transport in graphene are presented. They are deduced as moment equations of the semiclassical Boltzmann equation with the needed closure relations obtained by resorting to the Maximum Entropy Principle. The models differ in the choice of the moments to assume as basic field variables. A comparison is performed with the results given by directly solving the transport equation. For low and moderate electric fields, both models are reasonably acceptable but it has been found out that it is crucial to include, among the variables, the deviatoric part of the stress tensor in order to maintain a good accuracy in a wider range of applied electric fields. For each model, both linear and non-linear closure relations have been considered. Apparently, the nonlinearity does not improve the results.

NOTES

Active Forcing as a Non-Equilibrium Environment for Brownian Motion: Fluctuation Theorem and Mutual Information

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We consider a Brownian particle which, in addition to being in contact with a thermal bath, is driven by active fluctuations. These active fluctuations do not fulfil a fluctuation–dissipation relation and therefore play the role of a non-equilibrium environment. Using an Ornstein–Uhlenbeck process as a model for the active fluctuations, we derive the path probability of the Brownian particle subject to both, thermal and active noise. From the case of passive Brownian motion, it is well-known that the log-ratio of path probabilities for observing a certain particle trajectory forward in time versus observing its time-reserved twin trajectory quantifies the entropy production in the thermal environment. We calculate this path probability ratio for active Brownian motion and derive a generalized "entropy production", which fulfills an integral fluctuation theorem. We show that those parts of this "entropy production", which are different from the usual dissipation of heat in the thermal environment, can be associated with the mutual information between the particle trajectory and the history of the non-equilibrium environment.

NOTES

Temperature-Dependent Spectra and the Thermodynamics of Small Systems

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The energy and entropy of a small system are quantized, and so is the rate of change of one with respect to the other. Yet, when a small system comes into contact with a heat reservoir, its temperature adopts the reservoir's value. Using Elcock's and Landsberg's theory of temperature-dependent energy levels [*Proc. Phys. Soc., London, Sect. B*, 70, 161 (1957)], we propose an equilibration mechanism where the small system's temperature gradually approaches the reservoir's temperature in a non-trivial fashion, much like a bouncing ball approaches the ground before completely settling. This approach [*J. Phys. Chem. B*, 121, 10429 (2017)] produces standard thermodynamic results without invoking system size, offering an alternative view of the thermodynamic limit as a time-limit. It also provides a thermostatistical basis to the *thermodynamics of small systems* devised by Hill in the early 1960s [*J. Chem. Phys.,* 36, 3182 (1962); *J. Phys. Chem. B*, 120, 9180 (2016)].

NOTES

Gaussian Operations for Work Extraction and Storage

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One of the most fundamental tasks in quantum thermodynamics is extracting energy from one quantum system and subsequently storing this energy in an appropriate battery. Both of these steps, work extraction and battery charging, can be viewed as cyclic Hamiltonian processes realized by unitary transformations acting locally on a quantum system. While there exist so-called passive states whose average energy cannot be lowered by unitary transformations, it is safe to assume that the energy of any not-fully charged (quantum) battery may be increased unitarily. Nonetheless, unitaries raising the average energy by the same amount may differ in qualities such as their precision, fluctuations, and charging power, which one wishes to optimize. However, while work may be extracted from non-passive states in principle and optimal ways may be found of charging any specific battery, the required unitaries may be complicated and extremely difficult to realize in practice, in particular, in infinite-dimensional Hilbert spaces. It is hence of crucial importance to understand the qualities that can be expected from practically implementable transformations. In this talk, I will discuss the limitations for work extraction [1] and battery charging [2] when restricting operations on quantum harmonic oscillators to the arguably simplest and usually feasibly realizable family of Gaussian unitaries.

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NOTES

Abstracts

Session 2. Statistical Physics and Bayesian Computation

Fundamental Limits on the Thermodynamics of Circuits

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The thermodynamics of computation specifies the minimal entropy increase in the environment of any physical system that implements a given computation, when there are no constraints on how the system operates (the so-called Landauer limit). However common engineered computers use digital circuits to implement computations. The circuits topology introduces constraints on how the physical system implementing the computation can operate. These constraints cause additional minimal entropy increase, beyond that caused by the individual gates.

Here, we analyze this additional entropy increase, which we call circuit Landauer cost. We also analyze a second kind of circuit cost, which we call circuit mismatch cost. This is the extra entropy that is generated if a physical circuit that achieves minimal entropy production for a particular distribution q over its inputs is instead used with an input distribution p that differs from q.

We show that whereas circuit Landauer cost cannot be negative, circuits can have a positive or negative mismatch cost. In fact, the total entropy increase can be either increased or decreased by implementing a particular computation with a particular circuit. Furthermore, in general different circuits computing the same Boolean function have both different Landauer costs and different mismatch costs. This provides a new set of issues, never before considered, concerning how to design a circuit to implement a given computation with minimal thermodynamic cost. As a first step in analyzing these issues, we use tools from circuit complexity theory to analyze the scaling of thermodynamic costs for different computational tasks.

NOTES

The Entropy Production Paradox for Fractional Diffusion

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Fractional diffusion equations are an often used tool to describe anomalous diffusion observed in a variety of systems. However, apart from providing a successful basis for modelling such processes, fractional diffusion equations (sometimes also called fractional diffusion-wave-equations) show a fascinating property which makes them quite unique: They provide a one-parameter group of diffusion equations which allows a continuous transition from the dissipative classical diffusion equation to the reversible wave equation. This bridge between a fully irreversible and a fully reversible evolution equation shows a phenomenon which is known as the *Entropy Production Paradox*: as one moves from diffusion to wave behavior, the entropy production rate increases rather than decreases. This counter-intuitive property occurs for time- as well as space-fractional diffusion equations and not only for the Shannon entropy but also for the Tsallis- and Rényi entropies. We here review the known results and extend the analysis to a new type of fractional diffusion equation for which the solutions no longer possess the scaling properties used so far.

NOTES

Emergence of Tsallis Statistics as a Consequence of Invariance

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One of the most ubiquitous statistical distributions for non-equilibrium, steady-state systems is known as the q-canonical ensemble. Systems described by q-canonical distributions are common in Nature, for example, as non-equilibrium steady states in plasmas, fluids under turbulence, astrophysical systems (where gravitational interactions are dominant) and high-energy collisions [1–5]. A fundamental problem for the statistical physics of these steady states is to explain the origin of the non-canonical distributions. In 1988, Constantino Tsallis proposed a generalization of Boltzmann–Gibbs statistical mechanics (now known as non-extensive statistical mechanics), in which instead of the Gibbs–Shannon entropy one maximizes the generalized entropy Sq subjected to constraints [6]. After Tsallis'work, q is known as the non-extensivity parameter or entropic index, and the q-canonical statistics as Tsallis statistics. More recently, alternative mechanisms for producing q-canonical ensembles have been proposed, most prominently the idea of Superstatistics [7], which considers a system on a superposition of canonical ensembles described by a probability distribution of (inverse) temperatures.In this work, we present an alternative derivation of q-canonical ensembles, based on conditions of invariance requirements over the definition of subsystem and environment, and over the joint rescaling of temperature and energy. Our approach does not require theconcepts of Superstatistics or Tsallis statistics, but can be complementary to them.

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NOTES

Bayesian Approach with Local Regularization for Solving Reconstruction Problems

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From a rigorous mathematical point of view, a reconstruction problem is classified as an inverse and ill-posed one. The solution methods of this class of problems are defined by the term “regularization”. In general, regularization is the introduction of an a priori assumption about the problem in order to obtain a well behaved inverse. A fundamental problem of prior probability formulation in the Bayesian Maximum a Posteriori (MAP) approach is discussed in this paper. In standard MAP algorithms developed for Positron Emission Tomography (PET) and Single Photon Emission Computer Tomography (SPECT), one uses the prior based on the Gibbs model that results in global regularization. Global regularization, in which a single parameter controls the solution in the whole solution’s area, leads to the problems of edges over-smoothing and a loss of fine structures in reconstructed images. Both of these problems are very negative for PET and SPECT images, especially in oncology where the source function to be reconstructed is looking for high-gradient ‘hot spots’. The new approach with entropy prior which is based on the open system theory is presented in this paper. It is shown that this approach expanded the limits of the Gibbs prior and allowed to justify the method of local statistical regularization for PET and SPECT imaging. To test the approach, the SPECT of a source function with ‘hot spots’ is simulated. The results have shown that the hot spots were confidently reconstructed by using the MAP algorithm with local regularization, but they were practically lost in the images reconstructed by the standard algorithms with global regularization.

Acknowledgments: This work was partly supported by RFBR (grant No. 17-52-14004).

NOTES

The Entropy of a Classical Ideal Gas Whose Distribution Speed Law Is a Stretched Exponential Function

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The thermodynamic properties of a classical ideal gas can be derived from the microscopic approach in statistical mechanics. The equation of state is given by PV = NkT and the speed distribution law is given by a Gaussian function called the Maxwell–Boltzmann density. However, such an equation of state can be derived from a non-Gaussian density or stretched exponential function for ideal gases. This density is one for which its kinetic energy is power-law speed dependent with a given parameter. The corresponding Maxwell–Boltzmann density is recovered as a limit when the parameter (the exponent of the speed) of the power law is equal to 2. These kinds of densities are relevant in the study of granular gases, complex fluids and non-Gaussian relaxation processes. In this work, we study how the entropy of a non-Gaussian ideal gas deviates from the entropy of the Maxwell–Boltzmann case and its consequences for the corresponding thermodynamics properties.

NOTES

Abstracts

Session 3. Geometrical Science of Information, Topology and Metrics

Hyperbolicity of High Entropy Measures

Ali Tahzibi

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A deep analysis of the Lyapunov exponents—for a stationary sequence of matrices going back to Furstenberg; for more general linear cocycles by Ledrappier; generalized to the context of non-linear cocycles by Avila and Viana—gives an invariance principle for invariant measures with vanishing central exponents. In this talk, we give a new criterium formulated in terms of entropy for the invariance principle and in particular, obtain a simpler proof for some of the known invariance principle results.

As a byproduct, we study ergodic measures of partially hyperbolic diffeomorphisms whose center foliation is one-dimensional and forms a circle bundle. The project is to verify that, in generic setting, measures of high metric entropy have non-zero Lyapunov exponents, if the same holds for measures of maximal entropy. We show that for any such C2 diffeomorphism which is accessible, weak hyperbolicity of ergodic measures of high entropy implies that the system itself is of rotation type.

Acknowledgments: This is a joint work with J. Yang.

NOTES

Non-Linear Filtering and Entropy Production

Nina H. Amini

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Filtering theory gives an explicit model for the flow of information and thereby quantifies the rates of change of information supplied to and dissipated from the filter's memory. In this talk, we discuss the analysis carried out by Mitter and Newton for a linear case and also its extension to non-linear filters involving Markov diffusions. In particular, we can show that the central connection is made through the Mayer–Wolf and Zakai theorem for the rate of change of the mutual information between the filtered state and the observation history. Moreover, we extend this theorem to cover a Markov diffusion controlled by the observations process, which may be interpreted as the filter acting as a Maxwell's Dæmon applying feedback to the system. Here, we restrict our attention to a system where the state space is R^n; however, these results may be naturally extended to diffusions on manifolds under the usual technical assumptions derived by Schwartz and Meyer. Finally, we conclude this talk by presenting some possible extensions.
This talk is based on a joint work with John Gough (Aberystwyth University).

NOTES

Challenges in Non-Commutative Information Geometry

Jan Naudts

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Part of the recent work of (Montrucchio and Pistone, 2017) can be translated toa non-commutative context in a rather straightforward manner. This produces an example of what a theory of non-commutative deformed exponential families may look like and what the difficulties are due to non-commutativity. The present knowledge about Non-Commutative Information Geometry, as found in the book of (Petz, 2008), is reviewed. The recent work of (Montrucchio and Pistone, 2017) is situated in the context of Information Geometry. It considers the linear growth case of non-parametrizeddeformed exponential families (Naudts, 2004, 2011). Next, this work is generalized to the context of state vectors which are cyclic and separating for a given von Neumann algebra. The main result is a characterization of tangent planes. A parallel transport similar to that of the commutative case connects classes of tangent planes. J. Naudts, Estimators, escort probabilities, and phi-exponential families in statistical physics, J. Ineq. Pure Appl. Math. 5, 102 (2004). J. Naudts, Generalised Thermo statistics (Springer, 2011). L. Montrucchio, G. Pistone, Deformed exponential bundle: The linear growth case, in: Geometric Science of Information, GSI 2017 LNCS proceedings, F. Nielsen and F. Barbaresco eds., (Springer, 2017), p. 239-246; arXiv:1709.01430Dénes Petz, Quantum Information Theory and Quantum Statistics(Springer, 2008).

NOTES

Information Scan of Quantum States Based on Entropy–Power Uncertainty Relations

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In this talk, I will use the concept of entropy power to derive a new one-parameter class of information–theoretic uncertainty relations for pairs of observables in an infinite dimensional Hilbert space. This class constitutes an infinite tower of higher-order cumulant uncertainty relations, which allows in principle the underlying distribution to be reconstructed in a process that is analogous to quantum state tomography. I will illustrate the power of the new class by studying unbalanced cat states and the Cauchy-type heavy-tailed wave function that are of practical interest in quantum metrology. I will also briefly discuss the connection with generalized Cramer–Rao inequalities and De Bruijn's identity. Finally, I will try to cast some fresh light on the black hole information paradox.

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NOTES

Information Geometry in Classical and Quantum Systems

Eun-jin Kim

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A probabilistic description is essential for understanding the dynamics of stochastic systems far from equilibrium, given uncertainty inherent in the systems. To compare different Probability Density Functions (PDFs), it is extremely useful to quantify the difference among different PDFs by assigning an appropriate metric to probability such that the distance increases with the difference between the two PDFs. This metric structure then provides a key link between stochastic systems and information geometry. For a non-equilibrium process, we define an infinitesimal distance at any time by comparing two PDFs at times infinitesimally apart and sum these distances in time. The total distance along the trajectory of the system quantifies the total number of different states that the system undergoes in time and is called the information length. By using this concept, we investigate the information geometry of non-equilibrium processes involved in classical linear and nonlinear processes, governed by the Langevin equations. We then show that the information length proves to be valuable in measuring the information change as a quantum system continuously evolves in time. In particular, we elucidated consequences of quantum effects (uncertainty relation, energy quantisation) and the dual role of the width of PDF in quantum systems (PDF width can either increase or decrease the information length).

NOTES

Far-From-Equilibrium Time Evolution between Two Gamma Distributions

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Many systems in nature and laboratories are far from equilibrium and exhibit significant fluctuations, invalidating the key assumptions of small fluctuations and short memory time in or near equilibrium. A full knowledge of Probability Distribution Functions (PDFs), especially time-dependent PDFs, becomes essential in understanding far-from-equilibrium processes. We consider a stochastic logistic model with multiplicative noise, which has gamma distributions as stationary PDFs. We numerically solve the transient relaxation problem and show that as the strength of the stochastic noise increases, the time-dependent PDFs increasingly deviate from gamma distributions. For sufficiently strong noise, a transition occurs whereby the PDF never reaches a stationary state, but instead, forms a peak that becomes ever more narrowly concentrated at the origin. The addition of an arbitrarily small amount of additive noise regularizes these solutions and re-establishes the existence of stationary solutions. In addition to diagnostic quantities such as mean value, standard deviation, skewness and kurtosis, the transitions between different solutions are analysed in terms of entropy and information length, the total number of statistically-distinguishable states that a system passes through in time.

NOTES

Topological Information Data Analysis: Statistical Physic of Complex Systems, Application to Genetic Landscapes

Pierre Baudot, Monica Tapia, Jean-Marc Goaillard

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We establish methods that quantify the statistical interactions structure within a given data set using the characterization of information theory in cohomology by finite methods, and provide their expression in terms of statistical physics and machine learning.

Following previous work, we show directly that k-multivariate mutual-informations (I_k) are k-coboundaries. The k-cocycles, given by $I_k = 0$ generalize statistical independence to arbitrary dimension k.

We develop the computationally tractable subcase of simplicial information cohomology represented by entropy H_k and information I_k landscapes. The marginal I_1 component defines an internal energy U_k, and $(-1)^k$ $I_{k,k>1}$ components, the contribution to a free energy G_k of the k-body interactions. The set of information paths in simplicial structure is in bijection with the symmetric group and random processes, provides a topological expression of the second law, and points toward a discrete Noether theorem (first law). The local minima of free-energy, related to conditional-information negativity (non-Shannonian cone), characterize a minimum free energy complex. This complex formalizes the minimum free-energy principle in topology, provides a definition of a complex system, and characterizes a multiplicity of local minima that can account for the diversity observed in biology. It is computed by an algorithm called the Poincaré–Shannon machine and approximated by free software.

Finite data size effects severely constrain the computation of the information topology on data, and we provide a simple statistical test for the undersampling bias and for the k-dependencies. The application to genetic expression and cell-type classification recovers the known differential expressions and co-regulations of genetic modules, giving a topological version of Waddington epigenetic landscapes that quantifies the epigenetic information storage and learning beyond pairwise-interactions. This method provides tools for biological and ecological studies, and new methods of topological data analysis intrinsically based on statistics. This is joint work with Goaillard and Tapia.

NOTES

Hamilton–Jacobi Approach to Potential Functions in Information Geometry

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In this contribution, we want to analyze the problem of finding a potential function for a statistical manifold from an unconventional point of view. We will formulate the problem in a geometric and dynamical framework common to both the classical and quantum setting, and we will show that a solution of the Hamilton–Jacobi problem for a canonically defined Lagrangian L is actually a potential function for a given statistical manifold M. We point out that this formulation of the problem does not depend on the fact that M is a statistical manifold in the sense of information geometry, that is, our formulation can be naturally applied to cases in which the metric tensor on M is not the classical Fisher–Rao metric. The results presented here suggest that it could be possible to think of well-known divergence functions, such as the Kullback–Leibler divergence, as the Hamilton principal function of some suitable Lagrangian.

NOTES

Jean-Louis Koszul and the Hessian Information Geometry

Michel Nguiffo Boyom

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Let (Mo,Do) be a universal covering of an m-dimensional locally flat manifold (M,D) and let Q be the developing map of (M,D); Q is an affine immersion of (Mo,Do) which is the m-dimensional euclidean space. (M,D) is called a hyperbolic locally flat manifold after (Kaup–Koszul) if Q(Mo) is an open convex subset not containing any straight line. The Koszul Geometry is the geometry of locally flat hyperbolic manifolds. This Koszul Geometry has many strong connections with applied mathematics, information geometry and thermodynamics. It also has connections with the geometry of bounded domains. The first International Conference on Information Geometry took place in Ecole des Mines de Paris, in 2013. The plenary talk on 29 August was dedicated to Professor Jean-Louis Koszul who honored GSI 2013 by attending many talks on 29 August 2013. Thereafter, his interest in Hessian information geometry grew. The aim of my talk is to focus on some relevant commentaries of Professor Jean-Louis Koszul from 2013 to 2016. This talk is a homage to Professor Jean-Louis Koszul who left us on 12 January 2018.

NOTES

Sequential Structures of Statistical Manifolds

Hiroshi Matsuzoe

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A statistical manifold is a Riemannian manifold with mutually dual torsion-free affine connections. It is known that a parametric statistical model naturally has a statistical manifold structure. In the case of an exponential family, such a statistical manifold is reduced to a Hessian manifold. In recent years, anomalous statistics has been rapidly developing, and deformed exponential families play important roles in these statistics. A deformed exponential family naturally admits at least three kinds of statistical manifold structures, and one of them is not Hessian type.
From the viewpoint of unbiasedness of estimating functions, a deformed exponential family admits a sequential structure of expectations. As a consequence, one can obtain a sequence of statistical manifolds.
In this talk, we consider this sequential structure of statistical manifolds. We focus on not only Hessian structures of statistical manifolds, but also generalized conformal properties of statistical manifolds. In particular, alpha-conformal equivalence relations and conformal–projective equivalence relations are important in our framework.

NOTES

Abstracts

Session 4: Maximum Entropy Principle and Inference

Maximum Relative Entropy Parameter Estimation for a Dynamical System with Macroscopic and Microscopic Information Constraints

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When modelling dynamic processes from real world phenomena, we are often confronted with the problem that while the physics may suggest some general understanding regarding the form of the dynamical system, the specific details of the dynamical system may not be known to us. However, it is this form that we believe governs the production of measured data to which we have access. Besides the uncertainty in the form, these systems can often involve both extremely large amounts of data and be defined by an enormous amount of parameters, or very little data with few parameters. To deal with large complexity or little data, I propose using a method that can include relevant *macroscopic* of global information in addition to the data.

In practice, there are three "sizes" of systems: Large or *macro*scopic systems that can be adequately described by macroscopic information such as sample averages or using techniques such as mean field theory. Small or *micro*scopic systems that can be adequately described by microscopic information such as data and use Bayesian methods. However, the third size is in between such systems and which we will call mesoscopic systems. These systems can be too large for Bayesian methods due to complexity or time needed for computation, but are too small to use only macroscopic information where the fluctuations are too large in the sample averages.

Two toy examples will be shown. A noisy Lorenz system and a predator prey model where we wish to determine the parameters governing the system. We are assuming that this information is dynamic and may not come from the 'past' but is an 'active' constraint on the system.

NOTES

Maximum Entropy Analysis of Electrical, Water and Transport Networks

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The concept of a "flow network"—a set of nodes connected by flow paths—unites many different disciplines, including electrical, pipe flow, fluid flow, transportation, chemical reaction, ecological, epidemiological and human social networks. Traditionally, flow networks have been analysed by conservation (Kirchhoff's) laws and (in some systems) by network mappings (e.g., Tellegen's theorem), and more recently by dynamical simulation and optimisation methods. A less well explored approach, however, is the use of Jaynes' maximum entropy (MaxEnt) method, in which an entropy—defined over the total uncertainty in the network—is maximised subject to constraints, to infer the state of the network. We present a generalised MaxEnt framework to infer the state of a flow network, subject to "observable" constraints on expectations of various parameters, "physical" constraints such as conservation laws and frictional properties, and "graphical" constraints arising from uncertainty in the network structure itself. The method invokes an entropy defined over all uncertainties within the system, and infers a probability density function which expresses the (probabilistic) state of the network. In many instances, this framework requires new numerical methods for the iterative solution of systems with nonlinear constraints.

The analysis is demonstrated by application to a variety of systems, including (1) pipe flow networks, including a 1140-pipe urban water distribution network in Torrens, Australian Capital Territory, subject to nonlinear frictional constraints; (2) electrical networks—using a complex phasor formulation—including a 327-node urban electrical power distribution system in Campbell, Australian Capital Territory, with distributed power sources; and (3) three different transport network formulations, which incorporate trip, path and/or link flows, and various methods for route assignment.

NOTES

Information Geometry under Monotone Embedding

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The standard model of information geometry, expressed as a Fisher–Rao metric and Amari–Chensov tensor, reflects an embedding of probability density by log-transform.
The present paper studies parametrized statistical models and the induced geometry using arbitrary embedding functions, comparing single function approaches (Eguchi's U-embedding and Naudts deformed-log or phi-embedding) and a two-function embedding approach (Zhang's conjugate rho–tau embedding). While conjugate rho–tau embedding results in the most general form of divergence and cross-entropy of two probability density functions, the deformed-log and equivalently U-embedding give the most general form of entropy of a probability density function. In terms of geometry, the rho-tau embedding of a parametric statistical model defines both a Riemannian metric, called "rho–tau metric", and an alpha family of rho–tau connections, with the former controlled by one function \psi = 1/ (\rho^\prime \tau^\prime) and the latter by both embedding functions \rho and \tau in general. We identify conditions under which the rho–tau metric becomes Hessian and hence the +1/−1 rho–tau connections are dually flat. With respect to the \phi-exponential family, we demonstrated that the selection of (i) \psi = \phi renders the rho–tau metric Hessian, which is conformally equivalent to the metric derived from escort expectations. (ii) \psi= \phi / \phi^\prime renders the rho–tau metric conformallhy equivalent to the Tsallis metric obtained from a normalization function.
The previous case is realized, for instance, when either \rho or \tau is the identity, whereas the latter case corresponds to selecting \rho = \log_\tau or \tau = \log_\rho. Finally, we show a formulation of the maximum entropy framework which yields the phi-exponential family as the solution in both types of gauges.

NOTES

Entropy Unifies Ecology and Evolution

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Macroecologists study assemblages of differing species in communities, while evolutionary biologists study variants of heritable information within those species, such as DNA and epigenetics. Ecology and evolution share four basic processes—dispersal, random change, adaptation, and generation of novelty (speciation, mutation, and recombination)—but the fields differ in their approach to these. Although maximum entropy has been used in macroecology, this field often documents patterns without seeking underlying processes. On the other hand, evolutionary biologists have a long history of deriving and testing mathematical models, focusing on entropies such as Gini–Simpson and more recently Shannon, as well as their associated diversity measures within and between areas. Macroecology has borrowed these predictions for Gini–Simpson, and developed them further, but sometimes these methods have shortcomings. In the last decade, predictive equations have been derived for molecular diversity based on Shannon and mutual information. These equations are ready for use in macroecology also, which will allow analysis of a complete diversity “q-profile” in ecology and evolution, and provide information/entropy as a general predictive approach. Finally, the use of these methods will allow seamless integration with other studies such as the physical environment, and may even extend to assist with evolutionary programming in AI.

NOTES

Properties and Inequalities for ϕ-Entropies Derived from Inverse MaxEnt Problems

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This paper focuses on ϕ-entropy functionals derived from a MaxEnt inverse problem. This consists in determining an entropy, given a target maximum entropy distribution and given (usually simple) moment constraints. This kind of problem, considered, e.g., by Kesavan (1989), complements the usual maxent inverse problem where one looks for the constraints that will lead to a target maxent distribution, given the entropy. This approach allows distributions to be considered outside the exponential family—to which the maximizers of the Shannon entropy belong, and also to consider simple moment constraints, which can be estimated from the observed sample. We generalize Kesavan's approach and express the solutions and their properties in a broad setting. Our approach also yields entropic functionals that are functions of both probability density and state, allowing us to include skew-symmetric or multimodal distributions in the setting.
In the classical setting, there is an interplay between information measures (entropy, Fisher information) and moments. Associated to the generalized ϕ-entropies with a prescribed maxen distribution, we introduce informational quantities such as a generalized escort distribution, generalized moments and generalized Fisher information. These generalized informational quantities then allow the usual informational relations to be extended such as the Cram\'er-Rao inequality and the de Bruijn identity, relations saturated (or valid) precisely for the generalized MaxEnt distributions. Of course, classical results for Shannon and Rényi–Tsallis entropies are included as special cases.

NOTES

Entropy and Relevance among Questions

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Logical statements can be unambiguously ordered, more accurately, partially-ordered, according to whether one logical statement implies another. This is the Boolean algebra (lattice) of logical statements. Probability theory arises when one introduces a measure quantifying the degree to which one logical statement implies another. The familiar sum and product rules of probability theory serve to enforce consistency with basic symmetries: associativity of the logical OR and associativity of chaining inferences.

Logical questions can be similarly ordered (partially-ordered) based on whether one question answers, or resolves, another. Questions have been shown to form a partition sublattice (subalgebra) of the Free Distributive lattice (free distributive algebra). Analogous to probabilities, one can define a quantity that measures the degree to which one question answers another, which we call relevance. Relevance has analogous sum and product rules that arise from the symmetries shared by all lattices. By considering the relevance of a question to be a function of the probabilities of the statements that answer it, one can show that the relevance is proportional to the entropy of the set of possible answers. In fact, relevance can be shown to be proportional to the ratios of two entropies.

As a result, Shannon's information theory is recovered along with a calculus of entropy ratios. This question-based foundation reveals the fact that Shannon's entropy and information has a far broader domain of applicability than the communication channels for which it was originally developed.

NOTES

In Search of the Optimal Genetic Code: "What Does the Information Theory Have to Say about Evolution?"

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Nature uses a fixed genetic code which is one of the more than 10^{64} possible genetic codes. How did it choose this particular one? Is it optimal? Can we construct artificial genetic codes which are "better" than the natural genetic code? We start by answering the question "how do we measure the goodness of a genetic code?". We use Shannon Theory to model the protein coding process as an information transfer or communication process. We assert that better codes should have better information preserving capabilities and quantify the information-preserving capability during evolution with the channel capacity where the channel noise is characterised by mutations. We look into various mutation models and we calculate the channel capacity of both the non-coding RNA and the coding DNA where we consider a codon to the amino acid channel. We show that higher information capacity codes exist when compared to the natural genetic code and we design a machine learning algorithm to search for the optimal code. Although a good code, nature seems to have missed the optimal code. The results provide intuitions into the primordial code preceding the natural genetic code which seems to have been frozen at some point as Crick hypothesized. Is it plausible that codons were once composed of only two nucleotides instead of three? We also provide words of caution regarding our assumptions on the objectives of nature.

NOTES

Consistency of the Maximum Entropy Principle for Generalized Entropies

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The maximum entropy principle, originally formulated by E. T. Jaynes, provides a connection between thermodynamics and the theory of statistical estimation. As an inference method, the principle has been widely used in connection with Shannon entropy. In recent decades, many generalizations of Shannon entropy have appeared in thermodynamic applications. A natural question is whether these entropies can be utilized for the Maximum entropy principle and whether this inference method fulfills some logical consistency requirements. These requirements were formulated by Shore and Johnson [1]. Recently, several authors addressed this problem with different results [2–4]. We show that the class of the entropies fulfilling the Shore–Johnson consistency axioms consists of a large class of entropies [5], including the famous examples of Rényi entropy, Tsallis entropy or Sharma-Mittal entropy. They can be divided into equivalence classes of the entropy power functionals, depending on a single parameter q. We show that the parameter $q > 0$ is connected to the correlations of the resulting MaxEnt distributions of disjoint systems. The resulting distributions have the form of q-exponentials. For $q = 1$, we obtain ordinary MaxEnt based on Shannon entropy, leading to the independent MaxEnt distributions for disjoint systems. Finally, we show several applications of systems with intrinsic correlations, where the generalized Maximum entropy principle with $q \neq 1$. These examples include high-energy physics collisions or entangled quantum systems.

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NOTES

A New Signature of Quantum Phase Transitions from the Numerical Range

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One defining property of a quantum phase transition is a non-analytic ground energy in the thermodynamic limit of an infinite lattice model. We show for finite lattice models that the non-analyticity is related to the continuity of a maximum-entropy inference map and to the differential geometry of the domain of that inference map.

More precisely, we study the maximum-entropy inference map constrained on the two energy terms of a finite-dimensional one-parameter Hamiltonian. The domain of the inference map is the numerical range, a planar convex compact set.

The inference map is continuous if the energy terms of the Hamiltonian commute. In that case, the energy level curves are harmonic functions whose crossings fail to be C1 and the numerical range is a polytope. For non-commuting energy terms, it was known earlier but not stated explicitly that discontinuities of the inference map correspond to C1-smooth crossings of the ground energy with a higher energy level.

What is new in our contribution is the analysis of the boundary of the numerical range as a manifold (rather than an envelope). We show that the non-harmonic portions of the ground energy parametrize the curved boundary arcs of the numerical range, preserving the orders of smoothness at corresponding points. Hence, discontinuities of the inference map exist only at C1-smooth points of the boundary; these are C2-smooth or non-exposed points. Discontinuities exist at all C2-smooth non-analytic boundary points. Discontinuities at these points are essentially stronger than at analytic or non-exposed points.

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NOTES

Abstracts

Session 5: Kullback and Bayes or information theory and Bayesian inference

Optimization with Divergences

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For a long time, tight links have existed between information theory and optimization. Indeed, many problems encountered in information theory aim at minimizing or maximizing some relevant information measure (bitrate, capacity, distortion, etc.). We can mention in particular the celebrated Blahut–Arimoto alternating algorithm for minimizing mutual information under suitable linear constraints. In recent years, new bridges have been established between the two communities, revolving around optimization algorithms and phi-divergences. Two different research directions stand out. (1) Optimization for divergences. Divergences are constructed from perspective functions. As such, they possess some interesting convexity and lower semicontinuity properties, which allow them to be efficiently exploited in a wide range of nonsmooth optimization problems. In particular, proximal splitting methods can be employed to solve such problems, possibly under nonlinear constraints. One of the key problems in this context is the determination of the proximity operators of these divergences which play a prominent role in the implementation of these methods. (2) Divergences for optimization. The aforementioned proximal framework operates by building iteratively coercive surrogates to the terms appearing in a given objective function. Such a surrogate is classically obtained by adding a quadratic regularization to the function of interest. Alternative choices have been investigated in which the Euclidean metric is replaced by another notion of generalized distance, in particular a divergence. This has given rise to new algorithms whose convergence has been studied. In particular, these algorithms have been shown to be well-adapted to solving inverse problems involving some specific noise models, e.g., Poisson noise.

NOTES

Interactions of Information Transfer along Separable Causal Paths

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Complex systems arise as a result of inter-dependencies between multiple variables. Transfer entropy and information partitioning approaches have been used to characterize such dependencies. However, these approaches capture net information transfer occurring through a multitude of pathways involved in the interaction, and as a result mask our ability to discern the causal interaction within a subsystem of interest through specific pathways. We build on recent developments of momentary information transfer along causal paths proposed by Runge [Phys.Rev.E. 92, 062829 (2015)] to develop a framework for quantifying information partitioning along separable causal paths. Momentary information transfer along causal paths captures the amount of information transfer between any two variables lagged at two specific points in time. Our approach expands this concept to characterize the causal interaction in terms of synergistic, unique and redundant information transfer through separable causal paths. We analyze the impact of the separable and non-separable causal paths and the causality structure of the systems as well as the noises in the systems on information partitioning by using synthetic data generated from two coupled logistic equation models. Our approach can provide a valuable reference for an autonomous information partitioning along separable causal paths which form a subsystem.

NOTES

How Much Information Is Shared by Three Variables? Principled Generalizations of the Mutual Information to Three or More Variables

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In the years after Shannon published his seminal paper, "The Mathematical Theory of Communication," there were a number of efforts to extend his metric of redundancy between a pair of random variables to larger collections (Watanabe 1960, Fano 1961). The initial attempts to generalize the mutual information to ternary forms and beyond did not converge on a well-understood, standard set of measures, and in recent years, it has been demonstrated how these past approaches fail to effectively capture the notions of redundancy and causality (James and Crutchfield 2016, Schneidman, Bialek, and Berry 2003] that they are so often taken to represent. In recent years, researchers have proposed new measures that address some of these concerns (Williams and Beer 2011), but in this work we take a different approach by seeking information measures that capture a novel set of desirable properties that we would like our measure to satisfy. In addition to satisfying non-negativity and common-sense bounds when compared to the entropy and mutual information, we also require these measures satisfy a generalization of an important property respected by Shannon's mutual information: the Data Processing Inequality, which states that processing either of the variables cannot increase the information shared between them. Using these criteria, we have identified two new candidate measures of redundancy which modify Fano's original proposal: one derived from lattice theory which separates Fano's measure into a positive "redundancy" metric and negative "synergy" metric and another which obeys an additional additivity property. In addition to describing the measures, we examine their application to a few instructive examples and discuss their relevance to current debates in neuroscience.

NOTES

The Duality of Extropy/Entropy, and the Completion of the Kullback Information Complex

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The entropy measure of a probability mass function is entwined with a dual measure which is called extropy. The duality extends to the Kullback symmetric divergence which is the sum of two directed distances. I will display the dual equations, and exhibit a geometrical example in the two-dimensional unit simplex. Examining the equation that generates the symmetric measure as the sum of two directed distances, we will notice that the sum can be generated by two other pairs of functions as well. These are *not* any Bregman divergences, nor do they involve entropies or cross entropies at all. The Kullback information complex of four dimensions is intimately related to a proper score achieved by two distinct forecasting mass functions on the basis of an observation of the quantity concerned, the total logarithmic score. It is isomorphic to the expectations that the two forecasting distributions assess for their achieved scores, each for its own score and for the score achieved by the other. Analysis of the scoring problem exposes a Pareto optimal exchange of the forecasters' scores for assessing the quality of the information they provide regarding the observation. If there is time, I will exhibit a graphical example comparing the Pareto exchange scores to the direct proper scores in the assessment of this issue. The results are strikingly different.

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NOTES

Separating Diffuse from Point-Like Sources—A Bayesian Approach

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We present a method to separate superimposed point sources from auto-correlated, diffuse flux in images using a Bayesian model. A common problem, e.g., in astronomical imaging, is the superposition of bright, point-like sources and faint diffuse emissions. Separating stars from diffuse emission is of physical interest as the physical processes involved in each have to be studied individually to develop an understanding. The separation is an ill-posed problem with double the degrees of freedom than data points. It can be achieved only by considering additional information about the defining characteristics of the components in the form of prior knowledge. Point sources are by definition independently scattered in space. The diffuse emission exhibits strong spatial correlation, but a priori this correlation structure is not directly known in many cases. In our approach, we choose a log-normal model that enforces the positivity of the underlying density and allows for variation in the order of magnitudes, both intrinsically related to diffuse structures in the sky. The covariance structure of the diffuse emission prior is learned along the realization. For the point sources, we assume an inverse gamma prior with no spatial correlation. Those assumptions are used to build a fully Bayesian model, which allows the fast and reliable separation of the two components. We demonstrate the capabilities of the derived method on synthetic data and real data obtained by the Hubble Space Telescope.

NOTES

Abstracts

Session 6. Entropy in Action (Applications)

Biophysical and Biomedical Applications of the Gibbs Entropy Postulate

Jose M. G. Vilar

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The Gibbs entropy postulate is a cornerstone of mesoscopic non-equilibrium thermodynamics. I will discuss its general applicability to a wide diversity of systems that depart from the traditional local equilibrium assumption. I will consider physical processes, such as inertial effects in diffusion, as well as biomedical applications, including the characterization of leukemia on multidimensional morphological and molecular landscapes.

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NOTES

On Minimum Entropy and Gaussian Transport

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A nontrivial linear mixture of independent random variables of fixed entropies has minimum entropy only for Gaussian distributions. This "minimum entropy principle" was first stated for two variables by Shannon in 1948 in the form of the entropy-power inequality which has long been proven useful for deriving converse multiuser coding theorems. It was also also applied to deconvolution problems by Donoho and generalized to linear transformations by Zamir and Feder, and more recently to Rényi entropies with different formulations by Bobkov and Chistyakov and by Ram and Sason. Available proofs involve either the integration over a path of Gaussian perturbation of Fisher information or minimum mean-squared errors, or a limiting case of Young's convolutional inequality with sharp constants. In this work, we show that a natural transportation argument from the Gaussian distribution yields simple derivations of the minimum entropy principle in all these cases. The basic ingredient is a change of variable in differential entropies which dates back to Shannon's 1948 paper. We discuss possible generalizations and perspectives of this method.

NOTES

Temporal Information Partitioning Networks Reveal Ecohydrologic Responses to Rainfall Pulses and Drought

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Ecohydrologic fluxes within atmosphere, canopy and soil systems exhibit complex and joint variability. This complexity arises from direct and indirect forcing and feedback interactions that can cause fluctuations to propagate between water, energy, and nutrient fluxes at various time scales. When an ecosystem is perturbed in the form of a single storm event, an accumulating drought, or changes in climate and land cover, this aspect of joint variability may dictate responsiveness and resilience of the entire system. A characterization of the time-dependent and multivariate connectivity between processes, fluxes, and states is necessary to identify and understand these aspects of ecohydrologic systems. We construct Temporal Information Partitioning Networks (TIPNets), based on information theory and information decomposition measures, to identify time-dependencies between variables measured at flux towers along elevation and climate gradients in relation to their responses to moisture-related perturbations. Along a flux tower transect in the Reynolds Creek Critical Zone Observatory (CZO) in Idaho, we detect a significant network response to a large 2015 dry season rainfall event that enhances microbial respiration and latent heat fluxes. At a transect in the Southern Sierra CZO in California, we explore network properties in relation to drought responses from 2011 to 2015. We find that high and low elevation sites exhibit decreased connectivity between atmospheric and soil variables and latent heat fluxes, but the high elevation site is less sensitive to this altered connectivity in terms of average monthly heat fluxes. This work presents a novel use of information theoretic measures to gauge the responsiveness of ecosystem fluxes to shifts in connectivity, and aids our understanding of ecohydrologic responses to disturbances. This study is relevant to ecosystem resilience under a changing climate, and can lead to a greater understanding of shifting behaviors in many types of complex systems.

NOTES

Multiscale Weighted Permutation Entropy Analysis of the EEG in Early Stage Alzheimer Patients

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The aim of this study is to analyze the electroencephalography (EEG) of patients with mild Alzheimer's Disease (AD) while they were engaged in a memory task, and to contrast these results with those from cognitively Healthy Control subjects (HC). To do this, a novel extended version of the Multiscale Permutation Entropy (MPE), the MultiscaleWeighted Permutation Entropy (MWPE) method is introduced. This method is applied to the EEG signal of a large cohort of patients and controls during task execution. This allows comparison between the two groups of the complexity of the underlying brain signals at multiple temporal scales. Compared with the HC, the AD group exhibits a significantly decreased complexity in both the left and right central hemispheres, over courser temporal scales (5–7). These complexity results are then correlated with cognitive behavioral measures obtained during the memory task, to evaluate the correspondence between complexity and cognitive performance. In both the left and right central hemispheres, there exists a significant correlation. These results suggest that the MPE and the MWPE may be useful biological markers in AD patients.

NOTES

Particle Manipulation and Sorting by Entropy

David Reguera

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Confinement plays a very important role in many physical and biological systems. The diffusion of particles in zeolites and in microfluidic devices, the motion of biomolecules in the interior of a living cell or through ion channels, or the translocation of viral DNA into a cell, are examples where the evolution of the system is influenced by the tortuosity of a bounded region.

In this talk, I will discuss how these systems can be effectively described by introducing the concept of an entropic potential. We will see how the peculiar nature of entropic barriers has important and counterintuitive consequences in particle transport. In particular, phenomena such as entropic stochastic resonance, diffusion enhancement, and rectification take place in these systems and can be controlled by a smart application of external forces. These mechanisms can be used to optimize transport in confined media and for the manipulation and control of single molecules. In particular, I will discuss how the interplay of entropy, noise, and asymmetry can be used in an efficient separation mechanism that induces motion of particles of different sizes in opposite directions. This entropic splitting effect can be optimized for practical purposes and could be implemented in narrow channels and microfluidic devices.

NOTES

Entropy as an Indicator of Damage in Engineering Materials

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To estimate the extent of degradation, damage and life expended, an empirically based approach, called Physics of Failure (PoF), has been recently used to enhance the traditional statistical and probabilistic-based techniques of reliability and integrity assessment of critical structures and systems. In this research, a new approach in PoF analysis that relies on entropy as a more appropriate index of degradation and failure is discussed. For example, considering the irreversible thermodynamics, it is natural to conclude that entropy generated due to energy dissipation associated with all degradation mechanisms, such as fatigue cracking and corrosion, is a better index of materials damage. In this context, irrespective of the rate of entropy generation, material failure occurs when the cumulative entropy generated reaches a critical level, called entropic endurance to failure. Therefore, the second law of thermodynamics and entropy provide a strong foundation for describing failure and survival in materials. In this paper, three measures of estimating generated entropy, namely thermodynamic, information, and statistical mechanics entropies, will be explored and compared. The theoretical foundation of these entropic measures of materials damage will be discussed and demonstrated experimentally. Specifically, experimental results from fatigue damage of metallic specimens will be presented in the context of an entropic PoF model used to predict the extent of cumulative damage and remaining useful life of materials, by monitoring mechanical strain energy and thermal energy dissipations, and by inferring damage from the information entropy content of the cumulative fatigue damage generated by acoustic emissions.

NOTES

Estimation of the Number Density of Configurational Microstates in Steady-State Two-Phase Flows in Model Porous Media

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Steady-state two-phase flow in porous media is a process whereby a wetting phase displaces a non-wetting phase within a network of pores. The process is critical in many industrial, energy, environmental and biological applications. It is an off-equilibrium stationary process—in the sense that it is maintained in dynamic equilibrium at the expense of continuous energy supply to the system. The efficiency of the process depends on its spontaneity, measurable by the rate of global entropy production. The latter has been proposed to comprise two components: the rate of mechanical energy dissipation at constant temperature (a thermal entropy component, Q/T, in the continuum mechanics scale) and the configurational entropy (a Boltzmann–Gibbs entropy component, klnW), due to the existence of a canonical ensemble of flow configurations, physically admissible to the externally imposed macro-state conditions.

A recently developed analytical model (Valavanides and Daras, 2016 *Entropy* 18) implements a combinatorial analysis to evaluate the number of microstates per physically admissible internal flow arrangement. In particular, an analytical expression for counting the number of microstates, lnW, is delivered by contriving an appropriate mixing scheme over the canonical ensemble of the physically admissible flow configurations.

Nevertheless, implementation of the aforementioned B-G analytical expression demands knowledge of the individual physically admissible solutions of the entire ensemble. These are detected by a numerical scheme, based on a true-to-mechanism, stochastic pore-to-field scale-up model (DeProF). The latter scans the phase space on a voxel-partitioning scheme. In the present work, we deliver the transformation /equivalence between the virtual number of microstates estimated by the voxel-partitioning numerical scheme and the actual number of microstates over the continuum phase space of the actual flow. Indicative computations for a Berea sandstone model pore network are furnished.

NOTES

Fluctuation of Information Entropy Measures in a Cell Image

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The Biophysical Interdisciplinary Schottenstein Center for the Research and Technology of the Cellome, Physics Department, Bar Ilan University, Ramat-Gan, Israel

We introduce a simple, label-free cytometry technique, based on analysis of the random fluctuation of image Gray Level Information Entropy (GLIE), in order to reflect intracellular physiological and biophysical properties.

The intracellular medium could be characterized as a steady state, non-equilibrium, thermodynamic system with visco-elastic properties that enables correlation between intracellular diffusivity and generalized thermodynamic entropy.

The analytical relation between cellular diffusivity and thermodynamic entropy with regard to GLIE fluctuation measured in images of cells is explored.

For experimental evaluation of GLIE fluctuation, a combination of common bright field microscopy and a unique imaging dish wherein cells are individually held untethered in a picoliter volume matrix of optical chambers was used.

Experiments, simulation and theoretical examination have demonstrated that the SD of the information entropy function, when operating on image gray value fluctuation, is indifferent to microscope system “noise”.

The increase in intracellular diffusivity relates to elevated GLIE fluctuation by dowel synergic mechanisms. This important phenomenon leads to a clear advantage for the use of information entropy function to monitor intracellular fluctuation and diffusivity.

The ability of GLIE fluctuation measures to reflect basic cellular entropy conditions of early death and malignancy was demonstrated in a cell model of human, healthy–donor lymphocytes and malignant Jurkat cells, as well as dead lymphocytes and Jurkat cells.

As expected, GLIE fluctuations were greater in malignant Jurkat cells than in normal lymphocytes, and even more so, when compared to early dead cells.

Utilization of information entropy fluctuation measures to analyze cells in multiple physiological and pathophysiological conditions has an advantage in that it displays the biophysical characterization of tested cells, such as diffusivity and entropy, in a simple, unique and illustrative way.

NOTES

Maximum Entropy PDF Projection: Applications in Machine Learning

Paul Baggenstoss

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Recent work in the field of machine learning concerns two opposing types of networks: feed-forward networks including classical neural networks and deep neural networks (DNNs) which are deterministic, dimension-reducing networks; generative networks such as Bayesian and deep belief networks (DBNs), which are stochastic, dimension-increasing networks. Using maximum entropy PDF projection (MEPP), which is based on the the principle of maximum entropy, it is shown that there exists a unique generative model corresponding to each feed-forward network. This result has exciting ramifications because it indicates that the two forms of networks are, in fact, duals. In this talk, MEPP is reviewed, and the duality between feed-forward networks and generative networks is detailed. Applications of the duality are presented, and finally a classification experiment is presented in which feed-forward networks serve as generative networks, and can even compete with state-of-the-art deep belief networks in the classification of handwritten characters.

NOTES

A Kullback–Leibler Divergence Measure of Intermittency: Application to Turbulence

Carlos Granero-Belinchon, Stephane G. Roux, Nicolas B. Garnier

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We propose a new tool to analyze multifractality and intermittency. Our framework is based on information theory, and uses Shannon entropy and Kullback–Leibler divergence to measure the deformation of a probability density function across scales, from Gaussian at large scales to non-Gaussian at smaller scales.

In order to illustrate the performance of our new approach, we perform an extensive analysis of fully developed turbulence, the paradigmatic complex system where intermittency was historically defined. We describe our measure using both experimental Eulerian velocity measurements and synthetic processes, as well as a phenomenological model of fluid turbulence. We show that the Kullback–Leibler divergence characterizes the multifractal properties of a system so accurately that it is able to quantitatively discriminate predictions of various models which were previously indistinguishable. Compared to traditional measures of intermittency, like the flatness or the scaling exponents, our approach thus appears as the finest available. Moreover, it is model-free, as it does not rely on any assumption on the distributions and their specific evolutions across scales, so it can be directly applicable to a wide class of systems, such as physical, biological or social.

NOTES

Change-Point Detection Using the Conditional Entropy of Ordinal Patterns

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Ordinal time series analysis with the central concept of Permutation entropy is a relatively new approach to investigating long and complex time series. The idea behind it is to consider the order relation between the values of a time series instead of the values themselves. This leads to ordinal patterns describing the local up and down in a time series. Distributions of ordinal patterns obtained are the base of a statistical analysis. Here, we discuss change-point detection on the base of ordinal time series analysis. For this, a statistic built on the conditional entropy of ordinal patterns being a conditional variant of Permutation entropy is introduced and investigated. The statistic quantifying local differences between ordinal pattern distributions requires only minimal a priori information on given data and shows good performance in numerical experiments. In particular, we give some theoretical background for justifying our method and demonstrate the application of the method to EEG data.

NOTES

Dynamical Entropy Measures to Diagnose Deficits in Mouse Spatial Exploration Behaviour

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Deficits in spatial memory and spatial exploration behaviour are symptomatic of Alzheimer's Disease, and are observed in many mouse models of the disorder. Altered spatial dynamics are visible in 2D tracking data while mice perform open field or corridor-based tasks. In order to automate aspects of the search for therapeutic approaches for neurodegenerative diseases, it would be useful to quantify these changes in spatial behaviour. Such a measure would additionally assist in the development of new spatial behaviour paradigms, such as head-fixed behaviour in virtual reality or flat, real-world environments, by allowing quantitative reference to free behaviour. We propose the use of the Shannon permutation entropy versus statistical complexity (H x C) plane for this purpose. We apply this approach to data recorded from freely moving mice exploring an open field, and to head-fixed mice navigating on a flat, air-suspended platform. We analyse data from wild type mice as well as from APP23 and 5xFAD mouse models of amyloidopathy, concluding that the approach is sufficiently sensitive to be useful in the analysis of their behavioural phenotypes.

NOTES

Prediction of Protein Configurational Entropy (Popcoen)

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Minimizing a suitable free energy expression G is arguably the most common approach in (ab initio) protein structure prediction where the achieved accuracy depends crucially on the quality of G. Nevertheless, one mayor contribution of the free energy, configurational entropy, is basically always neglected in G because its determination requires sampling of many configurations which is computationally too expensive for most applications. This praxis, however, can lead to incorrect results as configurational entropy has a major impact on the native state selection of proteins [1].
Here, we suggest a knowledge-based approach for incorporating configurational entropy [2] which is extremely fast as it does not involve any type of sampling. Instead, entropy is predicted with an artificial neural network which was trained on simulation data [3] of ~1000 representative proteins. The method is freely available as a server application (called Popcoen) allowing to easily incorporate configurational entropy into existing protein software. This can yield a significant performance increase as we show exemplarily for a prominent protein software tool (FoldX [4]).

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NOTES

Entropy in Statistical Sound and Vibration: From Macroscopic to Super-Macroscopic World

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We present a discussion on the physical meaning of a statistical theory of sound and vibration, called statistical energy analysis (SEA). SEA is a simple theory of sound and vibration that applies when the vibrational energy is sufficiently disordered. We introduce the main result of SEA called Lyon's law: the vibrational power exchanged between two vibrating subsystems is proportional to the difference of the modal energies. We highlight the analogy of Lyon's law with Clausius' principle in thermics by properly introducing a notion of 'vibrational temperature'. This is not the classical temperature of thermodynamics but the 'vibrational temperature' follows the same rules as classical temperature. Since Clausius' principle applies to that new notion of temperature, we show that SEA is nothing but a thermodynamical theory of sound and vibration. We further investigate the notion of entropy in this context and we discuss its meaning. We show that 'vibrational entropy' is a measure of information lost in the passage from the wave theory of sound and vibration and SEA, its thermodynamical counterpart. The situation is therefore similar to that of statistical physics which describes the passage from a microscopic world (at the scale of molecules or atoms) to a macroscopic world (beyond the mean-free-path), the exception being that the passage is now from a macroscopic world (at the scale of acoustical wavelength) to a disordered super-macroscopic world (at the scale of large rooms or structures).

NOTES

Abstracts

Special Session. Fourier 250th Birthday: Geometric Theory of Thermodynamics

A Variational Formulation for the Nonequilibrium Thermodynamics of Open Systems

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We propose a variational formulation for the nonequilibrium thermodynamics of open systems, i.e., systems which can exchange matter and heat with the exterior. The formulation is an extension of Hamilton's principle of classical mechanics that allows the inclusion of irreversible phenomena and exchanges with the exterior. The irreversibility is encoded into a nonlinear constraint given by the expression of the entropy production associated to all the irreversible processes involved. Our approach is based on the new concept of thermodynamic displacement. We illustrate our theory by presenting examples of open systems experiencing mechanical interactions, as well as internal diffusion, internal heat transfer, and their cross-effects. Our approach yields a systematic way to derive the complete evolution equations for the open system, including the expression of the internal entropy production of the system, independent of its complexity. It might be especially useful for the study of the nonequilibrium thermodynamics of biophysical systems.

NOTES

Dirac Structures, Interconnections, and Variational Formulations in Non-equilibrium Thermodynamics

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The notion of Dirac structures has been known as a useful modeling tool which enables us to understand complicated physical systems such as nonholonomic mechanics, electric networks, and second-order fluids through the interconnection structure of energy conversion. In this talk, we study the Dirac structures that appeared in the discrete systems of nonequilibrium thermodynamics to show how the interconnection structure in nonholonomic mechanics can be extended to the case of nonequilibrium thermodynamics, where the phenomenological and associated variational constraints are encoded into nonlinear nonholonomic constraints. In particular, we demonstrate how our theory of the Dirac formulation is constructed consistently with the Hamilton–Pontryagin variational formulations for both thermodynamic Lagrangians and Hamiltonians in the generalized context of nonlinear nonholonomic mechanics. Our approach completely yields the first and second laws as well as the evolution equations. We illustrate our approach by treating several systems such as adiabatic pistons, membranes with mass transfer, etc.

NOTES

On the Contact Geometry and the Poisson Geometry of the Ideal Gas

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We elaborate on existing notions of contact geometry and Poisson geometry as applied to the classical ideal gas. Specifically, we observe that it is possible to describe its dynamics using a three-dimensional contact submanifold of the standard five-dimensional contact manifold used in the literature. This reflects the fact that the internal energy of the ideal gas depends exclusively on its temperature. We also present a Poisson algebra of thermodynamic operators for a quantum-like description of the classical ideal gas. The central element of this Poisson algebra is proportional to Boltzmann's constant. A Hilbert space of states is identified and a system of wave equations governing the wavefunction is found. Expectation values for the operators representing pressure, volume and temperature are found to satisfy the classical equations of state. We also analyse issues related to the (non)unitarity of the representation of thermodynamical observables by means of (non)Hermitean operators on Hilbert space.

NOTES

Riemannian Geometry of Fluctuation Theory: A Counterpart Approach of Information Geometry

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Fluctuation geometry was recently proposed as a counterpart approach to Riemannian geometry of inference theory (widely known as *information geometry*). This theory describes the geometric features of the statistical manifold $\mathcal{M}$ of random events that are described by a family of continuous distributions $\mathrm{dp}(\mathrm{x}|\theta)$. A main goal of this work is to clarify the statistical relevance of the Levi–Civita curvature tensor $\mathrm{R}_{\mathrm{ijkl}}(\mathrm{x}|\theta)$ of the statistical manifold $\mathcal{M}$. For this purpose, the notion of *irreducible statistical correlations*} is introduced. Specifically, a distribution $\mathrm{dp}(\mathrm{x}|\theta)$ exhibits irreducible statistical correlations if every distribution $\mathrm{dp}(\check{\mathrm{x}}|\theta)$ obtained from $\mathrm{dp}(\mathrm{x}|\theta)$ by considering a coordinate change $\check{\mathrm{x}} = \phi(\mathrm{x})$ cannot be factorized into independent distributions as $\mathrm{dp}(\check{\mathrm{x}}|\theta) = \prod_{\mathrm{i}} \mathrm{dp}^{(\mathrm{i})}\left(\check{\mathrm{x}}^{\mathrm{i}}\middle|\theta\right)$. It is shown that the curvature tensor $\mathrm{R}_{\mathrm{ijkl}}(\mathrm{x}|\theta)$ arises as a direct indicator of the existence of irreducible statistical correlations. Moreover, the curvature scalar $\mathrm{R}(\mathrm{x}|\theta)$ allows to introduce a criterium for the applicability of the *Gaussian approximation* of a given distribution function. This type of asymptotic result is obtained in the framework of the second-order geometric expansion of the distributions family $\mathrm{dp}(\mathrm{x}|\theta)$, which appears as a counterpart development of the high-order asymptotic theory of statistical estimation.
In physics, fluctuation geometry represents the mathematical apparatus of a Riemannian extension for Einstein's fluctuation theory of statistical mechanics. Some exact results of fluctuation geometry are now employed to derive the *invariant fluctuation theorems*. Moreover, the curvature scalar allows some asymptotic formulae to be expressed that account for the system fluctuating behavior beyond the Gaussian approximation, e.g., it appears as a second-order correction of Legendre transformation between thermodynamic potentials, $\mathrm{P}(\theta) = \theta_{\mathrm{i}}\bar{\mathrm{x}}^{\mathrm{i}} - \mathrm{s}(\bar{\mathrm{x}}|\theta) + \mathrm{k}^2\mathrm{R}(\mathrm{x}|\theta)/6$.

NOTES

Geometric Theory of Information and Heat Based on Souriau Lie Groups Thermodynamics for Machine Learning

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Best-In-Class data analytics algorithms are based on neural networks using both the natural gradient from information geometry and the stochastic gradient from the thermodynamical Langevin equation coupled with robust estimation of the Fisher matrix [1]. Jean-Marie Souriau has proposed to study the statistical mechanics from the new point of view of Symplectic geometry, completing the work of Poincaré and Cartan on integral invariant, reinventing the Lagrangian symplectic form in place of classical variational formulation and geometrizing the Noether Theorem with a moment map as new conserved quantities. Firstly, Souriau Lie Group Thermodynamics [2] gives geometrical status to the (Planck) temperature and the Entropy with a new general definition of the Fisher Metric. Secondly, Souriau Relativistic Thermodynamics of continua [3–5] provides a geometrization of the second principle by the permanence of the Entropy current, whose flux has positive divergence. For the case of a small data analytics, when Gibbs density is fluctuating, we have a generalized Souriau model introducing a polysymplectic generalization of Maximum entropy and Gibbs density in Lie Group Thermodynamics [6]. This Geometric theory of Heat allows us to generalize Information Geometry in more abstract spaces.

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NOTES

Abstracts

Poster Exhibition – Session 1

1. A Combinatorial Interpretation for Tsallis' 2-Entropy

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While Shannon's entropy is related to the exponential growth of multinomial coefficients, we show that Tsallis' 2-entropy is connected to their quantum version. When q is a prime power, these q-multinomial coefficients count the number of flags in F_q^n with prescribed length and dimensions (here F_q denotes the field of order q); in particular, the q-binomial coefficient $n\brack k$ counts vector subspaces of dimension k. Based on this idea, we obtain a combinatorial interpretation for non-additivity, as well as a frequentist justification for the maximum entropy principle with Tsallis statistics. We introduce a discrete-time stochastic process associated to the q-binomial distribution, that generates at time n a vector subspace of F_q^n. The concentration of measure around a "typical subspace" allows us to generalize some theorems by Shannon on source coding. Additionally, this process gives a very tractable example of exploding phase space (whose cardinality grows super-exponentially), recently discussed by Jensen, Pazuki, Pruessner and Tempesta.

2. A Derivation of a Microscopic Entropy and Time Irreversibility from the Discreteness of Timemik

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While the basic microscopic physical laws are time reversible, the arrow of time and time irreversibility appears only at the macroscopic physical laws by the second law of thermodynamics with its entropy term S. It is the attempt of the present work to bridge the microscopic physical world with its macroscopic one with an alternative approach to the statistical mechanics theory of Gibbs and Boltzmann. For simplicity, a “classical”, single particle in a one-dimensional space is selected. In addition, it is assumed that time is discrete with constant step size. As a consequence, time irreversibility at the microscopic level is obtained if the present force is of complex nature (not constant in time). In order to compare this discrete time irreversible mechanics with its classical Newton analog, time reversibility is reintroduced by scaling the time steps for any given time step n by the variable s(n), leading to the Nosé–Hoover Lagrangian comprising a term N*kB*T*ln(s(n)) (with kB the Boltzmann constant, T the temperature, and N the number of degrees of freedom) which is defined as the microscopic entropy Sn at time point n multiplied by T. Upon ensemble averaging of the microscopic entropy in a many-particles system in thermodynamic equilibrium, it approximates its macroscopic counterpart known from statistical mechanics. The presented derivation with the resulting analogy between the ensemble averaged microscopic entropy and its statistical mechanics analog suggests that the entropy term itself has its root not in statistical mechanics but rather in the discreteness of time.

3. A Model for Entropy Generation in Stagnation Point Flow of Non-Newtonian Jeffery, Maxwell and Oldroyd-B Nanofluids

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We present a single generalized model to describe the flow of three non-Newtonian nanofluids, namely, Jeffery, Maxwell and Oldroyd-B nanofluids. Using this model, we study entropy generation and heat transfer in the laminar boundary-layer stagnation point flow. The flow is subject to an external magnetic field. The conventional energy equation is modified by the incorporation of nanofluid Brownian motion and thermophoresis effects. A hydrodynamic slip velocity is used in the initial condition as a component of the entrenched stretching velocity. The system of nonlinear equations is solved numerically using three different methods, a spectral relaxation method, a spectral quasi-linearization method and the spectral local liberalization method, firstly to determine the most accurate of these methods, and secondly as a measure to validate the numerical simulations. The residual errors for each method are presented. The numerical results show that the spectral relaxation method is the most accurate of the three methods, and this method is used subsequently to investigate the empirical impact of the physical parameters on the fluid properties and entropy generation.

4. Entropy Generation of Casson Nanofluids over an Exponential Stretching Sheet with Non-Linear Thermal Radiation and Binary Chemical Reaction

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In this paper, we study the mixed convection entropy generation of Casson nanofluid over an exponential stretching sheet with non-linear thermal radiation, viscous dissipation, andbinary chemical reaction. A novel feature of this study is the investigation of entropy generation in a combined Casson nanofluid and the use of the recently developed spectralquasilinearization method (SQLM) to solve the conservation equations. This analysis is carried out in order to enhance the system performance. Convergence criteria are obtained graphically and numerically. Various fluid parameters of interest such as entropy generation, fluid velocity, shear stress heat and mass transfer rates are studied quantitatively and their behaviors are depicted graphically. Among the findings reported in this study is that the entropy generation has a significant impact in controlling the rate of heat transfer in the boundary layer region. The results also show that entropy generation increases with an increase in the Reynolds and Brinkman number.

5. Asymptotic Equivalence between Phase Space Volume Scaling of Generalized Entropies and Anomalous Diffusion Scaling Governed by Corresponding Non-linear Fokker-Planck Equations

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Many physical, biological or social systems are governed by history-dependent dynamics or are composed of strongly interacting units, showing an extreme diversity of microscopic behaviour. Macroscopically, however, they can be efficiently modeled by generalizing concepts of the theory of Markovian, ergodic and weakly interacting stochastic processes. In this paper, we model stochastic processes by a family of generalized Fokker-Planck equations whose stationary solutions are equivalent to the maximum entropy distributions according to generalized entropies. We show that at asymptotically large times and volumes, the scaling exponent of the anomalous diffusion process described by the generalized Fokker-Planck equation and the phase space volume scaling exponent of the generalized entropy objectively determine each other via a simple algebraic relation. This implies that these basic measures characterizing the transient and the stationary behaviour of the processes provide the same information regarding the asymptotic regime, and consequently, the classification of the processes given by these two exponents coincide.

6. Connecting Information Geometry to Geometric Mechanics

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We connect information geometry to geometric mechanics in an attempt to provide a unified framework for mechanics and information. It is well-known that, since the Hamiltonian dynamics is well captured by the symplectic flow in the cotangent bundle T*M, discretizing and representing the dynamics in the product manifold MxM preserves all dynamical information about the mechanical flow. We then compare the symplectic structure on MxM as induced by a divergence function in information geometry with the canonical symplectic structure on T*M that supports the Hamiltonian flow, and establish that any divergence function inducing a statistical structure can also serve as a generating function for the symplectic structure. Note that our identification of information geometry and geometric mechanics is via pull-back of the canonical symplectic form from T*M to MxM via a symplectomorphism specified by a divergence function; we have not used dynamics and geometric structures on the TM side. In fact, we propose to decouple the Lagrange dynamics (on the TM side) and the Hamiltonian dynamics (on the T*M side) for information systems, in distinction from their mandatory Legendre coupling in mechanical systems. (Work in collaboration with Melvin Leok.)

7. Connection between Continuum and Kinetic Theories: Application for Rarefied Gases

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The motivation to extend the classical laws such as Fourier and Navier–Stokes equations comes from the experiments. Regarding heat conduction in solids, the second sound is measured in superfluid He by Peshkov, then the ballistic propagation is detected in NaF crystals by Jackson et al. In parallel, the behavior of rarefied gases is investigated and it has also shown a phenomenon beyond the Navier–Stokes equation.

The common point between these experiments is related to the kinetic modeling of the transport phenomena: the question is the behavior of a rarefied gas in both cases but only the type of gas differs.

Our goal is to derive the continuum equations in the framework of non-equilibrium thermodynamics using internal variables and current multipliers. It is shown that the compatibility with the kinetic theory can be obtained through the proper generalization of entropy current. Moreover, the resulting system of constitutive equations is tested on experiments. First, the modeling of ballistic propagation in NaF crystals is presented. On the other hand, the experiments performed by Rhodes et al. are also analyzed. Finally, the results are compared with related ones based on Rational Extended Thermodynamics.

8. Eigenstate-Specific Temperatures in Two-Level Paramagnetic Spin Lattices: Obedience or Disobedience to the Third Law of Thermodynamics at Small *N*?

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The compatibility of four eigenstate-specific temperatures (ESTs) for "forward" ($j \geq j + 1$) and "reverse" ($j - 1 \geq j$) transitions in paramagnetic spin lattices (PSLs) with the Third Law of Thermodynamics is explored. Microcanonical and canonical ESTs defined as derivatives $(dU/dS)_V$ are designated "continuous"; microcanonical and canonical ESTs defined as finite difference ratios (delta$U$/delta$S$)$_V$ are designated "discrete".
When the Third Law is obeyed, the ESTs of the perfect crystalline ground ([n_{up}, n_{down}]) = [N, 0]) and maximum energy ([0, N]) eigenstates should both equal zero. Nevertheless, for forward transitions *from* the ground state, only T_c= 0 K for all N; the other three ESTs approach zero only in the large N limit. For forward transitions *from* the maximum energy state, T_c = 0 K for all N, and $T_u^{j \geq j+1}$ ≥ 0 K as N becomes large. However, T_{du} and T_{dc} are poorly defined because the entropy is imaginary for the *final* [–1, N + 1] state, which is non-physical. T_{du} and T_{dc} are likewise poorly defined for reverse transitions transitions *into* the ground state, because in this case the *initial* [N + 1, –1] state is non-physical. These results will be discussed in light of the Schottky heat capacity anomaly.

9. An Alternative Presentation of the Second Law of Thermodynamics

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We present an elementary, but still quite rigorous derivation of the Clausius inequality, which provides a new perspective on the second law. Unlike the classical approach, our derivation does not employ the Carnot cycle. The Clausius inequality follows in a straightforward way from the first law and thermodynamic stability conditions without invoking the Clausius or the Kelvin–Planck statement of the second law. The background knowledge required for this article is the same as that for the usual textbook presentation of the second law. The new presentation of the second law is, therefore, appropriate for an introductory thermodynamics course.

10. Entropy Production in Matter Aggregation Mesoscopic Phenomena with a Tour toward the Involvement of (Inter)Molecular Interactions

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Aggregation is a complex phenomenon in which various effects play a role. The competition amongst various types of interactions (electrostatic, hydrophobic, steric, van der Waals, etc.) results in different types of molecular aggregation. Building any model that explains these aggregation phenomena, one should have knowledge on the relative role of the various fundamental interactions in such systems and their real impact on the aggregation of molecules. Another, namely geometrical, property of molecular aggregates—their curvatures, uncovering in global vs. local ways their structures—also has a big impact on this phenomenon. These curvatures are associated with a suitable choice of physical (interaction expressing) potentials, governing the system. Interaction-driven aggregations can run in systems, which are out of thermodynamic equilibrium. These types of phenomena are well described by nonequilibrium, and often nonlinear thermodynamic formalisms. The description assumes that the thermodynamic state variables are in local equilibrium. Then, we use the fluxforce relations, with the Onsager coefficients, while ending ultimately at a local conservation law. This formalism works in the space of the grain sizes. The entropy production is then defined in terms of the aforementioned flux and its conjugated thermodynamic forces. In the presented work, we would like to address fluxes and forces in a picture of submesoscopic and intermolecular interaction-affected nonequilibrium thermodynamics. We will present analytical and numerical results revealing essential peculiarities of selected types of molecular aggregations, especially those based on colloid type viz amphiphilic self-assemblies as well as biomembranes, and their vesicles-involving counterparts. It turns out that any essential signatures of decisive intermolecular interactions, emanating from the submesoscopic soft-matter organisation level, find their clear embodiments at its truly mesoscopic counterpart.

11. Global Passivity in Microscopic Thermodynamics

Raam Uzdin

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With the rapid development of quantum technologies and the ability to manipulate individual atoms and ions, thermodynamics faces new challenges. Not only its validity is in question, but also its ability to provide useful predictions. The main thread that links classical thermodynamics and the thermodynamics of small quantum systems, is the celebrated Clausius inequality form of the second law. However, its application to small quantum systems suffers from two cardinal problems: (i) The Clausius inequality does not hold when the system and environment are initially correlated—a commonly encountered scenario in microscopic setups. (ii) In some other cases, the Clausius inequality holds, but does not provide any useful information (e.g., in dephasing scenarios). We address these deficiencies by developing the notion of global passivity and employing it as a tool for deriving thermodynamic bounds. Crucially, on top of the Clausius inequality, the present framework provides additional thermodynamics bounds that accompany the second law. To illustrate the role of the additional bounds, we use them to detect unaccounted heat leaks, and weak feedback operations ("Maxwell's demons") that the Clausius inequality cannot detect. In addition, global passivity sets practical upper and lower bounds on the buildup of system–environment correlation for dephasing environments. Our findings are relevant for experiments in various systems such as ion traps, superconducting circuits, atoms in an optical cavity and more. If time permits, the more general mathematical foundations of this framework, i.e., Bregman divergence and Schur concavity, will be discussed.

12. Hierarchical Structure of Generalized Thermodynamic Entropy

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The present research is aimed at outlining a method to generalize thermodynamic entropy property and characterize the hierarchical structure of the canonical definition at the macroscopic and microscopic level. The conceptual schema is based on dualisms and symmetries inherent to the geometric and kinematic configurations and interactions occurring in many-particle or few-particle thermodynamic systems. The hierarchical configuration of particles and sub-particles, constituting a system, breaks down levels characterized by particle masses subdivision, implying positions and velocity degrees of freedom multiplication. This hierarchy accommodates the propagation of phenomena and processes from higher to lower levels in the respect of the equipartition theorem of energy. However, the opposite and reversible process, from lower to higher levels, is impossible by virtue of Second Law, expressed as impossibility of Perpetual Motion Machine of the Second Kind (PMM2) remaining valid at all hierarchical levels, and the non-existence of Maxwell's demon. Based on the generalized definition of entropy property, the hierarchical structure of entropy contribution and production balance, determined by degrees of freedom and constraints of systems configuration, is established. Moreover, as a consequence of the Second Law, the non-equipartition theorem of entropy is enunciated, which would be complementary to the equipartition theorem of energy derived from the First Law.

13. Information Entropy of Liquid Metals

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Correlations reduce the configurational entropy of liquids substantially below their ideal gas limits. By means of first principles molecular dynamics simulations, we obtain accurate pair correlation functions, then subtract the mutual information content of these correlations from the ideal gas entropy to predict the entropy over a broad range of temperatures. Because the ideal gas entropy is derived from quantum mechanics, this method yields the absolute (third law) entropy. We apply this method to liquid aluminum and copper and demonstrate good agreement with experimental measurements, then we apply it to predict the entropy of a liquid aluminum–copper alloy. We find that the mixing entropy of the alloy nearly vanishes owing to strong short-ranged chemical order in the liquid state. Corrections due to electronic entropy and many-body correlations are discussed. Our results show that quantification of information provides a simple and convenient route to liquid metal entropy without requiring thermodynamic integration.

14. Magnetic Engine for the Single-Particle Landau Problem

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Quantum thermodynamics is one of the most interesting topics in physics today. The possibility to create an alternative and efficient nanoscale device, like its macroscopic counterpart, introduces the concept of the quantum heat engine, which was proposed by Scovil and Schultz-Dubois in the 1950s [1]. The key point is the quantum nature of the working substance and also the quantum version of thermodynamic laws. The combination of these two simple facts leads to very interesting studies of well-known macroscopic engines, such as Carnot, Stirling, and Otto, among others.

In our case, we study the effect of the degeneracy factor on the energy levels of the well-known one electron in a magnetic field (the Landau problem) for a magnetic engine, proposed previously [2]. The scheme of the cycle is composed of two adiabatic and two isomagnetic processes, driven by a quasi-static modulation of external magnetic field intensity. We derive the analytical expression of the relation between the magnetic field and temperature along the adiabatic process and reproduce the expression for the efficiency as a function of the compression ratio. In particular, we obtain a radically different behavior of the typical harmonic case and found that a major increase in the external magnetic field to reach the Carnot efficiency is necessary. We remark that the useful work of this engine, related to change in the magnetization along the process, can be used, for example, in the generation of induction current in other physical systems. In the near future, we will extend this work to include edge states and the many electrons scenario for a more realistic approach.

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15. Power and Efficiency Analysis of a Simplified Curzon–Ahlborn Engine

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In 1975, Curzon and Ahlborn (CA) [1] presented an expression for Efficiency at Maximum Power (EMP), modelling a thermal engine which consists of a Carnot-type cycle. In recent decades, a new branch of thermodynamics has emerged, known as Finite Time Thermodynamics (FTT). The model proposed by Curzon and Ahlborn operates between two heat sources with high and low temperatures, respectively, and the expression for the EMP obtained was, in principle, independent of the model parameters and only dependent on the temperatures of the heat reservoirs; analogously, this is what happens with the efficiency for a reversible Carnot cycle. However, to obtain the efficiency of CA, it is necessary to consider that the heat transfer involved obeys a linear law. Notice that, previously, others authors [2,3] have found the same expression for similar models. An important advantage observed in the results obtained in FTT is that the optimal efficiency values are closer to those observed in real engines [4]. Within the context of FTT, several objective functions to be optimized under rich criteria have been introduced and, many models of heat engines have been proposed and analyzed which perform as motors, heat pumps or refrigerators.

In this work, the optimal performance of a simplified Curzon–Ahlborn engine, proposed by Agrawal in 2009 [5], is studied; it has also been studied with Newton and Dulong–Petit heat transfer law by Páez-Hernández R et al. [6,7]. The performed analysis takes into account three operating regimes: Maximum Power, Maximum Ecological Regime and Efficient Power criterion. Results show analogies in the optimal performance between thermal and isothermal engine models.

16. Reconsidering the Foundations of Thermodynamics from an Engineering Perspective

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There were two paths to thermodynamics: the engineering path of the Carnots concerned with engines and efficiency, and the scientific path of Clausius concerned with describing the world. Their results are not compatible. Atkins: "Thermodynamics still has both aspects, and reflects complementary aims, attitudes, and applications."

I offer a Popperian 'bold hypothesis': engineering thermodynamics is the more general foundation wherein the scientific idealizations are special cases.

For Cardwell, the scientific account is a 'rational reconstruction'. Quantum theory is more general than all possible mechanics. Following Cardwell, I reconsider thermodynamics from a post-mechanical, quantum perspective.

My bold hypothesis requires a link between quantum theory and Carnot's engineering thermodynamics. What connects them is 'action', originally expressed in Maupertuis's principle of least action.

Maupertuis proposed 'action' to resolve the competing conservation principles based on mv and mv^2. Maupertuis's more general 'action framework' incorporated both complementary, conservation principles—challenging scientific 'objectivity'. The 'appropriate' mechanical-conservation frame of reference depends on the observer's frame of reference. To the surprise of the scientific fundamentalists, Maupertuis's indeterminate two-aspect 'action framework' re-emerges explicitly with Planck's quantum of action.

There is a disconnect between Sadi Carnot and Clausius. For engineer Carnot, work results from a cycle. Heat is always conserved: "This is a fact which has never been disputed." For Clausius, heat is consumed proportionally as work is performed. Plausibly, they are using different definitions of heat and work. Carnot's efficiency limit provides a quite different account of the impossibility of perpetual work and the arrow of time. Maupertuis's corresponding concern with evolution is not coincidental.

17. Testing Foundations of Quantum Mechanics at the Gran Sasso Underground Laboratory

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We will focus on the experimental investigation of two of the most fascinating items of QM: the measurement problem and the spin-statistics connection.
The first part of the talk will concern the study of the Dynamical Reduction Models (DRMs). The linear and unitary nature of the Schrödinger equation allows, in principle, for the superposition of states of macroscopic objects. The wave packet reduction principle avoids superpositions, but its stochastic nature contrasts the deterministic time evolution; the scale of the superposition breakdown is not overpredicted. DRMs consist of non-linear and stochastic modifications of the Shrödinger equation (containing new physical parameters) which induce a diffusion process for the state vector, responsible for the wave packet collapse. According to DRM models, charged particles emit radiation (spontaneous radiation) when interacting with the stochastic "collapsing" field. Results will be presented of dedicated measurements with a setup based on high purity, coaxial p-type Germanium detectors, conceived for the search of a spontaneous radiation signal from which the most stringent limits on the DRM parameters were obtained.

The second part will focus on the investigation of possible small violations of the Pauli Exclusion Principle (PEP) for electrons, through the search for "anomalous" X-ray transitions in copper atoms, produced by "new" electrons (brought inside a copper strip by circulating a current) which may undergo Pauli-forbidden transitions to the 1 s level already occupied by two electrons. The experimental results achieved by the VIP and the VIP2 upgrade experiments will be presented.

18. Thermodynamic Analysis of Irreversible Desiccant Systems

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A general thermodynamic analysis of desiccant systems is carried out in order to estimate the potentiality and the proper application field of this technology for certain target room conditions and given outdoor temperature and humidity. An expression of the entropy balance, suitable for describing the operability of a desiccant system at steady state, is obtained by applying a control volume approach, defining sensible and latent effectiveness parameters, and assuming ideal gas behaviour of the air–vapour mixture. This formulation, together with mass and energy balances, is used to carry out a general screening of the system performance. The theoretical advantage and limitation of the desiccant dehumidification air conditioning, the maximum efficiency for given conditions constraints, the least irreversible configuration for a given operative target, as well as the characteristics of the system for a target efficiency can be obtained. Once the thermo-physical properties and the thermodynamic equilibrium relationship of the desiccant mixture are known, this method can be applied to a specific technical case in order to select the most appropriate working fluid and guide the specific system design.

19. VIP2 at Gran Sasso—High Sensitivity Validity Test of the Spin Statistics Theorem for Electrons

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The VIP2 (VIolation of the Pauli Exclusion Principle) experiment at the Gran Sasso underground laboratory (LNGS)) is aiming at a high sensitivity search for possible violations of standard quantum mechanics predictions in atoms. With high precision, we investigate the Pauli Exclusion Principle and the collapse of the wave function (collapse models). We will present our experimental method of searching for possible small violations of the Pauli Exclusion Principle (PEP) for electrons, via the search for "anomalous" X-ray transitions in copper atoms, produced by "new" electrons which could be likely to undergo Pauli-forbidden transition to the ground state already occupied by two electrons. We will describe the VIP2 experiment, which is currently obtaining data at LNGS. The goal of VIP2 is to test the PEP for electrons with unprecedented accuracy, down to a limit in the probability that PEP is violated at the level of 10^{-31}. We will present current experimental results and discuss the implications of a possible violation.

Abstracts

Poster Exhibition – Session 2

20. Approximate Bayesian Computation for Estimating Parameters of the Data-Consistent Forbush Decrease Model

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Realistic modeling of complex physical phenomena is always quite a challenging task. The main problem usually concerns the uncertainties surrounding model input parameters, especially when not all information about a modeled phenomenon is known. In such cases, Approximate Bayesian Computation (ABC) methodology may be helpful. The ABC can be based on a comparison of the model output data with the experimental data, to estimate the best set of input parameters of the particular model.

In this paper, we present a framework applying the ABC methodology to create a realistic model of the Forbush decrease (Fd) of the galactic cosmic ray intensity. Fds are observed on Earth by the neutron monitors during the Sun increased activity periods. The Fd model requires the numerical solution of the Fokker–Planck equation in five-dimensional space (three spatial variables, the time and particles energy). The most problematic in Fd modeling is the lack of detailed knowledge about the spatial and temporal profiles of the parameters responsible for the creation of the Fd. Among these parameters, the diffusion coefficient plays a central role. Assessment of the correctness of the proposed model can be done simply by comparing the model output data with the experimental data of the galactic cosmic ray intensity.

We employ the Sequential Monte Carlo ABC algorithm, scanning the space of the diffusion coefficient parameters within the region of the heliosphere where the Fd is created. The proposed algorithm is adopted to create the model of the Fd observed by the neutron monitors on Earth in March 2002. The Fd model is based on the stochastic approach to the solution of the Fokker–Planck equation.

Abstracts

Poster Exhibition – Session 3

21. A Matrix Generalization of Relative Entropy and Entropy Power Inequalities

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This work proposes a matrix generalization of the relative entropy, also known as the Kullback–Leibler divergence. The proposed relative entropy matrix is defined as an integral over the signal-to-noise ratio of the excess mean square estimation error incurred by a mismatched estimator on a Gaussian channel. The trace of the matrix is equal to the classical relative entropy.

In the first part of the paper, properties of the matrix relative entropy are studied. In particular, it is shown that the new quantity is non-negative definite, is equal to zero if and only if the distributions agree, and is a convex operator on the space of distributions.

In the second part of the paper, it is shown that the proposed matrix relative entropy leads to matrix generalizations of entropy power inequalities (EPIs). In particular, new matrix versions of Lieb's inequality, Gaussian log–Sobolev inequality, and Zamir–Feder EPIs are shown. Moreover, the new matrix inequalities lead to a richer body of classical EPIs.

22. Harmonic Sierpinski Gasket and Applications

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The harmonic version of the Sierpinski gasket is analyzed with particular emphasis on the geodesic metric. In fact, noncommutative geometry can provide a natural metric on the fractal. In particular, Lapidus and Sarhad proved that the natural metric coincides with Kigami's geodesic metric. The most common and intuitive presentation of the Sierpinski gasket is that obtained from a solid equilateral triangle by the removal of inverted equilateral triangles. Topologically, it is well described analytically as the unique fixed point of a certain contraction mapping on a metric space. In particular, it can be generalized by the harmonic metric to become the geometric space called the harmonic gasket, that is the harmonic Sierpinski gasket. This present work extends the classical theory of the Sierpinski gasket. In addition, due to the wavelet analysis, new properties are given. Numerical simulations confirm the theoretical results. Some applications are given and discussed in detail.

23. 1-D versus 2-D Entropy Velocity Law for Water Discharge Assessment in a Rough Ditch

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The assessment of water discharge in open channel flow is one of the most crucial issues for hydraulic engineers in the fields of water resources management, river dynamics, eco-hydraulics, irrigation, hydraulic structure design, etc. Recent studies state that the entropy velocity law allows expeditive methodology for discharge estimation and rating curve development due to the simple mathematical formulation and implementation. Many works have been developed based on the 1-D formulation of the entropy velocity profile, supporting measurements in the lab and field for rating curve assessment but, in recent years, the 2-D formulation has been proposed and applied in the studies of regular ditch flows, showing a good performance. Present work deals with the comparison between the two 1-D and 2-D approaches in order to give a general framework of threats and opportunities related to robust operational application of such laws. The analysis has been carried out on a laboratory ditch with regular roughness, under controlled boundary conditions and different stages, generating an exhaustive dashboard for the better appraisal of the approaches

24. Algebraic Models of Hazard and Risk. Applications to Risk and Control Banding Tools

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Hazard and risk determine the probability of adverse outcomes. The classical model of risk is a mapping from the abstract space of events to the compact interval $[0,1]$ of probabilities. In practice, the risk can be estimated by counting the number of adverse outcomes. For rare events, however, this setting is not feasible. Such is also the case for the occupational hazards related to advanced materials, for example, in nanoform, where the novel engineered properties can bring unanticipated hazards. Hence, in such circumstances, one can expect the appearance of exceptional risk and uncertainty, which is difficult to account for in quantitative models. Assessment of risk needs only functionality for the risk or adverse outcomes to be graded. This understanding brought about tools, which only categorize different outcomes—the so-called risk and control banding tools. Despite their usefulness, there is little theoretical work dedicated to their operation. This contribution aims to present an algebraical foundation of the categorical risk assessment approaches. The minimal algebraic structure supporting such categorical inference is the ordered idempotent monoid M. Additionally, the risk classification can be defined as a function M to M. This structure encompasses all available control banding tools. The algebraic structure is implemented in the popular computer algebra system Maxima.

25. An Information Geometric Classification of Complex Systems Based on Generalized Entropies

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Using the generalized entropies which depend on two parameters, we propose a set of quantitative characteristics derived from the Information Geometry based on these entropies. Our aim, at this stage, is to first construct some fundamental geometric objects which will be used in the development of our geometrical framework. We first establish the existence of a two-parameter family of probability distributions. Using this family, we derive the associated metric and we state a generalized Cramer–Rao Inequality. This gives a first two-parameter classification of complex systems. Then, computing the scalar curvature of the information manifold, we obtain a further discrimination of the corresponding classes. We further construct a new information manifold which offers us the possibility to make some predictions of characteristic values of complex systems.

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26. Combining Entropy Measures for Anomaly Detection

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The combination of different sources of information is a problem that arises in several situations, for instance, when data can be compared using different similarity measures. Often, each source of information is given as a similarity/distance/kernel matrix. In this paper, we propose a new class of methods in order to produce, for anomaly detection purposes, a single Mercer kernel (that acts as a similarity measure) from a set of local entropy measures, related to Mercer kernels in the context of density estimation. This kernel is used to build an embedding of data in a variety that will allow the use of a (modified) one-class Support Vector Machine (SVM) to detect outliers. We study several information combination schemes and their limiting behaviour when the data sample size increases within an Information Geometry context. In particular, we study the variety of the given positive definite kernel matrices to obtain the desired kernel combination as belonging to that variety. The proposed methodology has been evaluated on a variety of real and artificial problems.

27. Entropic Renormalization Group Flows in Statistical Manifolds

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Renormalization Group (RG) methods have been instrumental in tackling problems involving an infinite number of degrees of freedom. There is a wide variety of versions of the RG. What they have in common is that they allow a systematic search for choosing the degrees of freedom that describe the information that is relevant to the phenomenon of interest. This suggests that an approach that emphasizes the connection to notions of information and entropy might be particularly valuable. Recently, such an exact RG has been developed as a form of Entropic Dynamics (*Entropy* *2018*, 20(1), 25). Since the transformations are infinitesimal, the formalism can be described as a continuous dynamical flow in a fictitious time parameter. It is generally the case that these RG equations are functional diffusion equations. In this paper, we further develop the Entropic RG formalism by studying the RG flow restricted to statistical submanifolds of finite dimension using techniques of information geometry.

28. Information Geometry of Qubit State Tomography

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It is well known that the Stokes parametrization $(\xi_1, \xi_2, \xi_3) \mapsto \frac{1}{2}(I + \xi_1\sigma_1 + \xi_2\sigma_2 + \xi_3\sigma_3)$, where $\{\sigma_i\}_{1\leq i\leq 3}$ are the standard Pauli matrices, establishes a one-to-one affine isomorphism between the state space of a two-level quantum system (qubit) and the unit ball (the Bloch ball) embedded in the three-dimensional Euclidean space. This fact sometimes misleads us to an incorrect picture that the qubit state space is also statistically isomorphic to the unit ball endowed with the Euclidean structure. In this study, we investigate the geometrical structure of the Bloch ball from an information geometrical point of view.

Suppose that, in the course of a qubit state tomography, the ith Pauli matrix σ_i was measured N_i times and obtained outcomes $+1$ (spin-up) and -1 (spin-down) n_i^+ times and n_i^- times, respectively. Then, the ambient space $(-1,1)^3$ of the Bloch ball is regarded as a Riemannian manifold endowed with a metric $g_{ij} := N_i\delta_{ij}/(1-(\xi_i)^2)$, and the maximum likelihood estimate is the orthogonal projection from the empirical distribution onto the Bloch ball along a geodesic with respect to the mixture connection.

29. Open Problems on Geometry of Information in Steady-State Two-Phase Flows in Pore Networks

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Steady-state two-phase flow in porous media is a process whereby a wetting phase displaces a non-wetting phase within a pore network. It is maintained in dynamic equilibrium at the expense of continuous energy supply to the system. Wettability, hydrodynamic flow instabilities and pore-scale disorder induce the disconnection of the non-wetting phase into small fluidic elements, incessantly exchanging position and momentum, as they migrate downstream at macroscopically constant flow rates under constant pressure gradients. The average macroscopic flow constitutes a hierarchical system, typically resulting in complex flow patterning and creating a dynamic mixture of repeating cycles of emerging spontaneous structures and cascading failures, restructuring, etc. In the mechanistic-stochastic DeProF model, flow is described by an ergodic ensemble of physically admissible configurations, consistent with the externally imposed macroscopic flow conditions. The ensemble is simply connected in the 3D phase space of flow configurations. It contains critical information on the process' interstitial structure. Its atypical shape characteristics change with flow conditions: from low to high intensity flows, starting from a small size, the ensemble swells and changes shape as its mass center follows a trajectory in phase space, before it shrinks back to a minimum size.

The information associated with the volume of the ensemble was directly correlated to the interstitial degrees of freedom of the process and its configurational entropy. Yet there is still much latent, untapped information within the first and higher-order moments, of the ensemble shape characteristics. An unresolved modeling problem is to properly implement ergodicity considering the ensemble shape characteristics. Ergodicity implies that all physically admissible flow configurations have equal probability of being visited by the process. Yet, as the shape of the ensemble is atypical (pebble, bean), the flow configurations residing in its central part would be visited more frequently than others residing in remote areas.

30. Spherical Minimum Description Length

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We consider the problem of model selection using the Minimum Description Length (MDL) criterion for distributions with parameters on the hyper sphere. Model selection algorithms aim to find a compromise between goodness of fit and model complexity. Variables often considered for complexity penalties involve number of parameters, sample size and shape of the parameter space, with the penalty term often referred to as stochastic complexity. Current model selection criteria either ignore the shape of the parameter space or incorrectly penalize the complexity of the model, largely because typical Laplace approximation techniques yield inaccurate results for curved spaces. We demonstrate how the use of a constrained Laplace approximation on the hyper sphere yields a novel complexity measure that more accurately reflects the geometry of these spherical parameters spaces. We refer to this modified model selection criterion as spherical MDL. As proof of concept, spherical MDL is used for bin selection in histogram density estimation, performing favorably against other model selection criteria.

31. Robust Geometric Means for Covariance Estimation with Heterogeneous Data

Yongqiang Cheng, Xiaoqiang Hua, Hao Wu, Hongqiang wang, Yuliang Qin

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This work explores the computations of geometric means, associated with six distances or divergences, of a set of Hermitian positive-definite (HPD) matrices. It is applicable to covariance estimation for heterogeneous data. In particular, several efficient means with analytical expressions are obtained. The problem of covariance estimation is reformulated as the geometric means of HPD matrices on a Riemannian manifold. Without resorting to the complete knowledge of probability distribution of the data, the geometry of the Riemannian manifold is considered in the mean estimator. Then, the performance of covariance estimation can be improved. Moreover, the robustness of geometric means is analyzed via the influence function of outliers. We find that the Kullback–Leibler mean exhibits the best robustness among these geometric means. The results show that the performance of an adaptive normalized matched filter with the proposed mean estimator outperforms the classical ones, especially in a contaminated clutter.

32. Total Jensen–Bregman Divergence on a Manifold of HPD Matrices with Applications to Radar Signal Processing

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A class of total Jensen–Bregman (tJB) divergence on a Riemannian manifold of Hermitian positive-definite matrices is presented, and is applied to deal with problems in radar signal processing. In particular, three tJB divergences, including total Jensen square loss, total Jensen log-determinant divergence, and total Jensen–von Neumann divergence, are obtained by choosing different forms of the convex function in the definition of tJB divergence. Their corresponding centroids are derived. Then, two applications of the proposed tJB divergence are considered: (1) design a matrix constant false alarm rate (CFAR) detector; (2) reformulate the covariance estimator in adaptive radar processing as the tJB centroid on a Riemannian manifold. In addition, the robustness of centroids is analyzed by adding outliers. The results show that the matrix CFAR detector with the tJB divergence has better performance than the Riemannian distance-based matrix CFAR detector, while the performance of an adaptive normalized matched filter with the tJB centroid outperforms the existing alternatives.

33. Types of Ricci Tensors in Submanifold Theory

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The problem of studying Einstein metrics of Riemannian manifolds is of great interest both for mathematicians and physicians. It is well known that real hypersurfaces in Hermitan symmetric spaces of rank one such as the complex projective and complex hyperbolic space, and of rank two such as the complex two-plane Grassmannians and the complex hyperbolic two-plane Grassmannians, do not admit the Einstein metric. The non-existence of Einstein real hypersurfaces results in the definition of new types of Ricci tensors on real hypersurfaces. We give new types of Ricci tensors defined on real hypersurfaces. The two new types of Ricci tensors are the *-Ricci tensor and the k-th generalized Tanaka–Webster Ricci tensor. We present results concerning the existence or non-existence of metrics satisfying geometric conditions similar to the condition of the Einstein metric and to the condition of Ricci soliton with respect to the new types of Ricci tensors. Potential applications of these metrics in physics are also provided.

Abstracts

Poster Exhibition – Session 4

34. Sufficiency of Bregman Divergences in Thermodynamic Systems

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If a physical system is in state s but we believe that the system is in state t, then one can define the divergence d(s,t) as the energy that could have been extracted if we knew that the system is in state s minus the energy that we can extract when we act as if the state was in state t. This definition d(s,t) is a so-called Bregman divergence. In the paper "Divergence and Sufficiency for Convex Optimization", *Entropy* 2017, 19(5), 206, it has been proved that if a system has a Bregman divergence that satisfies a sufficiency constraint, then the Bregman divergence is proportional to KL divergence so that the Bregman divergence is generated by the Shannon entropy. Similarly, for quantum systems, the result singles out quantum relative entropy that is the Bregman divergence generated by the von Neuman entropy. For a thermodynamic system, the sufficiency condition translates to the conservation of free energy under reversible processes. Nevertheless, the result cannot be applied directly because a physical process may be subjected to constraints such as the conservation of energy. In this lecture, we will see how to overcome this problem. We will also discuss the monotonicity of Bregman divergences that corresponds to a decrease of free energy under irreversible processes. Monotonicity implies sufficiency but, more surprising, sufficiency also implies monotonicity.

35. Admission Decision Using the Maximum Entropy Principle

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Admission exams often consist of several subjects such as mathematics, physics and essays. Then, the admission decision is based on a weighted sum of the scores. This kind of procedure is necessary in other situations such as rating of firms. Since the weight affects the decision, an objective weighting method is desired. We provide an algorithm using the maximum entropy principle such that the average score of each subject over the admitted people is greater than that over the rejected people, where borderline decisions should be randomized. Here, the entropy is maximized over the set of probability distributions that are obtained by coordinate-wise affine transformation of the given random vector and have a fixed expectation of a hinge-type function. The problem is reduced to a convex optimization problem with respect to the weight variables, and therefore is effectively solved. Numerical examples are presented to illustrate the properties of the method.

36. Discerning the Thermodynamic Basis of Self-Organization in Critical Zone Structure and Function

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Self-organization characterizes the spontaneous emergence of order. Self-organization in the Critical Zone, the region of Earth's skin from below the groundwater table to the top of the vegetation canopy, involves the interaction of biotic and abiotic processes occurring through a hierarchy of temporal and spatial scales. The self-organization is sustained through input of energy and material in an open system framework, and the resulting formations are called dissipative structures. Why do these local states of organization form and how are they thermodynamically favorable? We hypothesize that structure formation is linked to energy conversion and matter throughput rates across driving gradients. Furthermore, we predict that structures in the Critical Zone evolve based on local availability of nutrients, water, and energy. By considering ecosystems as open thermodynamic systems, we model and study the throughput signatures on short times scales to determine the origins and characteristics of ecosystem structure. This diagnostic approach allows us to use fluxes of matter and energy to understand the thermodynamic drivers of the system. By classifying the fluxes and dynamics in a system, we can identify patterns to determine the thermodynamic drivers for organized states. Additionally, studying the partitioning of nutrients, water and energy throughout ecosystems through dissipative structures will help identify reasons for structure shapes and how these shapes impact major Critical Zone functions.

37. Entropy Meets Bioinformatics: DNA Frequency Dictionaries and Beyond

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The frequency dictionary is a list of the strings of a given length that occur in DNA accompanied with their frequency. A relation between the dictionaries derived for the strings of different length is the key issue: as a rule, any given frequency dictionary is unambiguously transformed into the dictionary comprising shorter strings, while the inverse transformation is ambiguous. Invariant manifold methodology (adapted for symbol sequences) provides the unique expanded frequency dictionary (comprising longer strings) from a given one; that latter is the dictionary of the most expected continuations from the given set of strings. Such an expanded dictionary yields maximal entropy, over the ensemble of all admissible expansions. A comparison of the given frequency dictionary to the expanded one from the dictionary of shorter strings provides the information capacity of the given dictionary; mutual entropy (Kullback measure) is the way to compare them. A number of biological entities are considered, in terms of the information capacity. Additionally, the strings of increased information value are defined: these are the strings exhibiting greater deviation between the real frequency and the expected frequency. Also, an alignment-free method to compare symbol sequences is developed, based on a mutual entropy calculation of the frequency dictionaries of the group of entities under comparison, against the common statistical ancestor. That latter is the arithmetic mean of the given set of frequency dictionaries; remarkably, such a definition yields the minimum of the sum of mutual entropy figures of each frequency dictionary from the group under comparison, when calculated against the common statistical ancestor.

38. From Identity to Uniqueness: The Emergence of Increasingly Higher Levels of Hierarchy in the Matter Evolution Process

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A statistical interpretation of entropy was based on a model of ideal gas where point particles were considered as identical. The universe, on the contrary, from the very first second of its existence, has contained systems that consist of particles of different types: quarks and leptons; nucleons; nuclei; atoms; chemical compounds or monomers; heteropolymers; prokaryotes; eukaryotes, and multicellular organisms. Indeed, statistical entropy of these systems (when classical statistics began working) was greater than the entropy of ideal gas with the same number of particles due to the existence of several types of such particles. Afterwards, the number of such types in relation to the number of particles grew along the main hierarchical chain. On each level, statistical entropy that calculated by the Boltzmann formula: $S = K \ln W$ has an additional term that is equal to $K \ln (n! / \Sigma\, ni!)$ and becomes equal to $K \ln (n!)$ when all the particles are unique, i.e., the number of types is equal to the number of particles. Such uniqueness appeared in only ensembles of prokaryotes. Thus, hierarchogenesis adds a new aspect to the principle of maximum entropy: not only entropy itself increases up to its maximal value (for a given condition) but this maximum value itself increases at each level of the hierarchy. Herewith, there are different levels of uniqueness determined by the similarity of unique entities and the inverse dependence on redundancy of information that describes them. Indeed, algorithmic complexity, which is determined by a complete and minimal (i.e., not redundant) description of an entity, directly depends on this level of uniqueness. Thereby, jumps of an individual's uniqueness from prokaryotes to eukaryotes and then to multicellular organisms were accompanied by consecutive jumps of complexity according to the earlier-formulated general law of complification as generalization of the maximum entropy principle.

39. Jaynes' Entropy Principle for Quantum Markov Processes

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The Jaynes' maximum entropy principle provides a general method for how to infer probabilities from incomplete data. It has been applied to the analysis of many phenomena throughout various fields of science. In particular, the principle was found extremely successful in statistical physics, where it declares that an equilibrium state of a macroscopic system is characterized by the maximum of its entropy subjected to constrained mean values of given observables (usually constants of motion). The description of such states requires only a small number of parameters and these states take the form of a Gibbs state. Recently, it has been found that Gibbs states play an important role in the description of equilibrium quantum states also on smaller scales. However, whether in all or only certain situations and why the maximum entropy principle could be the proper paradigm for constructing the quantum equilibrium state remains rather unclear.

In our work, we study the equilibration process in the context of quantum Markov processes (including both discrete and continuous). For a broad class of quantum Markov processes, we identify their equilibrium states as well as their integrals of motion and prove that equilibration within quantum Markov processes follows the principle of minimum quantum relative entropy which coincides with the maximum entropy principle only for unital quantum Markov processes. Surprisingly, taking into account mutual algebraic relationships between equilibrium states and integrals of motion, one can show that all resulting equilibrium states can be cast into a generalized Gibbs state form and its partition function exhibits all the useful properties we are used to exploiting in statistical physics. Moreover, we show that eventual nonstationary asymptotic evolution is also governed by the similar Jaynes' principle.

40. Mean Variance-Weighted Entropy Approach to Portfolio Optimization

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Return and risk are key factors which need to be taken into account when constructing portfolio selection models. In addition to these factors, a third one, represented by liquidity, is of great relevance for investors. Entropy measures can be successfully used for the assessment of portfolio diversification, as a measure of liquidity. In this paper, new portfolio optimization models are constructed in the mean variance entropy framework. The optimal portfolio is obtained by maximizing a weighted combination of return and entropy under a given level of risk. The corresponding weights depend on the importance given by the investor to return and diversification. Several portfolio selection models are constructed using Shannon, weighted Shannon or parametric entropy measures. Analytical formulas for representing the solution of the portfolio optimization problem are obtained on the basis of this approach. A comparative analysis of the new models is performed and the properties of their solutions are investigated. Computational results are provided in order to prove the effectiveness of the proposed models.

41. Use of Finite Order Moments to Reconstruct the Langevin Equations by the Maximum Entropy Principle

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The Langevin equation (or stochastic differential equation) has been confirmed to be a powerful tool for modeling the dynamics of empirical systems with noise. While a noisy system should be described in terms of its probability distribution, an inverse question is how to construct the Langevin equation given that some finite order moments (such as mean, variance, etc.) of the system are known. Here, we introduce a comparison technique to address this issue. By assuming the detailed balance condition, the potential and noise terms of the Langevin equation can be constructed through a comparison of the corresponding coefficients. This procedure can construct a Langevin equation with nonequilibrium stationary distribution in accordance with the maximum entropy distribution subjected to the constraints of given moments. It offers a novel theoretical and numerical tool for treating Langevin dynamics occurring in physics, chemistry, biology and other diverse scientific fields. Moreover, the reconstruction is not unique and different Langevin equations can be constructed by the same constraints. Thus, we stress that the same maximum entropy distribution can result from systems with different dynamical behaviors.

Abstracts

Poster Exhibition – Session 5

42. Recent Developments in Information Field Dynamics

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Many simulation schemes for partial differential equations (PDEs)heuristically discretize individual differential operators or focus on minimizing a simple error norm of a discretized version of a field. Information field dynamics (IFD) takes a fundamentally different approach; the discretized field is interpreted as data providing information about areal physical field that is unknown. This information, given by the KL-divergence, is sought to be conserved by the scheme as the fieldevolves in time. We discuss recent advances of IFD for the problem of nonlinear PDEs in a noiseless Gaussian approximation. The Information loss serves as an action that can be minimized to obtain an informationally optimal simulation scheme. For the discussed case, the simulation scheme can be brought into a closed form using field operators to calculate the appearing Gaussian integrals. We present some results of applying resulting simulation schemes for the Burgers equation. Their accuracy surpasses finite-difference schemes on the same resolution. The IFD scheme, however, has to be correctly informed on the subgrid correlation structure. In certain limiting cases, we recover well-known simulation schemes such as spectral Fourier Galerkin methods.

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43. The Probability That an Unknown Number Is Greater Than a Known Number Is 1/2

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Reason compels us to treat two possibilities as equal in the absence of evidence to the contrary. This "principle of indifference" is the most fundamental and intuitive means of deriving probabilities from information. It is readily applied to spaces that have obvious symmetry, but it has appeared inapplicable with respect to asymmetrical spaces, such as positive numbers (e.g., distances). If we know only one positive number, is an unknown positive number more likely to be larger or smaller? Most numbers are larger than any known number. However, the principle of indifference suggests that larger and smaller are equally probable, and we prove this to be correct. Specifically, we prove that the median of a distribution over an unknown number conditional on a single known number is equal to the known number, for all cases in which joint distributions over positive real numbers are conditional on minimal information (exchangeability of variables and scale invariance). We further demonstrate that all logistic distributions, including the widely used logistic (sigmoid) function, are conditional on a single positive number. Our results advance the 'objective Bayesian' definition of probability and its application to cases of minimal information, including real-time prediction by neurons and other biophysical sensors.

44. A New Underwater Acoustic Signal Denoising Technique Based on CEEMDAN, Mutual Information, Permutation Entropy and Wavelet Threshold Denoising

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Owing to the complexity of the ocean background noise, underwater acoustic signal denoising is one of the hotspot problems in the field of underwater acoustic signal processing. In this paper, we propose a new technique for underwater acoustic signal denoising based on complete ensemble empirical mode decomposition with adaptive noise (CEEMDAN), mutual information (MI), permutation entropy (PE) and wavelet threshold denoising. CEEMDAN is an improved algorithm of empirical mode decomposition (EMD) and ensemble EMD (EEMD). First, CEEMDAN is employed to decompose noise signals into many intrinsic mode functions (IMFs). IMFs can be divided into three parts: noise IMFs, noise-dominant IMFs and real IMFs. Then, the noise IMFs can be identified on the basis of MIs of adjacent IMFs; the other two parts of IMFs can be distinguished based on the values of PE. Finally, noise IMFs were removed, and wavelet threshold denoising is applied to noise-dominant IMFs; we can obtain the final denoised signal by combining real IMFs and denoised noise-dominant IMFs. Simulation experiments were conducted by using synthesized data and a real underwater acoustic signal; the proposed denoising technique performs better than other existing denoising techniques, which is beneficial to the feature extraction of an underwater acoustic signal.

Abstracts

Poster Exhibition – Session 6

45. An Information Theoretic Approach to the Developing Auditory Brain

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A central goal of neuroscience is to understand how neurons in sensory regions of the cerebral cortex encode information about environmental stimuli. Classically, this has been approached by measuring the "receptive field" of a neuron: the average number of action potentials produced in response to some basic stimulus set. For example, one might examine how often an auditory neuron responds to a set of pure tones of varied frequency and speak of it being "tuned" to a "characteristic frequency." A hallmark of the developing brain is its heightened plasticity which is reflected in dynamic changes to these receptive fields. Despite several decades of studying receptive field properties, it is unknown whether they capture the stimulus information they are believed to encode. To address this, we applied an information theoretic approach to directly quantify the informativeness of neural activity in the developing brain. Previous research has established that the receptive field is sensitive to increasingly complex stimuli during development (Insanally et al. 2009); however, using the mutual information, we find that the encoding of simple stimuli present early on actually degrades as the brain adapts to represent more complex features. Furthermore, the Stimulus-Specific Information (Butts 2003, Montgomery and Wehr 2010) reveals that neurons are not always most informative about their characteristic frequency as is widely believed, and the correspondence also weakens over time. Finally, using Fano's measure of three-way redundancy, we show that distant neurons come to share a remarkable amount of stimulus information despite having entirely different receptive fields. These results demonstrate that information about simple sounds becomes less localized and salient in the developing auditory cortex. They also caution us to be careful when inferring functional significance directly from receptive fields and demonstrate the principled insights that can be gained by using tools from information theory to understand neuronal function.

46. Sample Entropy to Evaluate Atrial Fibrillation Pharmacological Cardioversion

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Atrial fibrillation (AF) is the most common arrhythmia in clinical practice and its prevalence is expected to rise dramatically, owing to an aging population. Pharmacological rhythm control is a treatment option for AF and the intravenous formulation of vernakalant has been approved for pharmacological cardioversion of recent-onset AF. This drug blocks the action potential of the channels of Na and K and extends the atrial refractory period without affecting only the ventricular.
A database is composed by atrial electrical activity signals extracted from surface ECG recordings from eight AF patients in different stages, during basal state and within 30 min of the infusion. Therefore, the evolution of atrial activity regularity is studied over time during the cardioversion procedure.
The results show a decrease of sample entropy atrial activity when the patients recover sinus rhythm with 0,116 ± 0.027 in basal state and 0.107 ± 0.024 after the vernakalant infusion, (p = 0.025). Moreover, it is possible to find two groups: one with a longest time until reversion to sinus rhythm, with a slow decrease of regularity over time, and a second with a higher decrease of the entropy in a shorter time.
These results confirm that an increase of regularity during AF is related with reversion to sinus rhythm.

47. A Novel Algorithm Based on the Pixel-Entropy for Lanes Detection and Lane Division Lines Formation

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Automatic lane detection for traffic surveillance in intelligent transportation systems is a challenge for vision-based systems. In this paper, *a novel pixel-entropy based algorithm for the detection of lanes and formation of their division lines* is proposed. Using as input a *video from a static camera*, each *pixel behavior in the gray color space* is modeled by a *time series*; then, for a time period τ, its histogram followed by *its entropy are calculated. Three different types of theoretical pixel-entropy behaviors* can be distinguished: *(1) the pixel-entropy at the lane center shows a high value; (2) the pixel-entropy at the lane division line shows a low value; (3) a pixel not belonging to the road has an entropy value close to zero.* From the road video, *several small rectangle areas* are captured, each with only a few full rows of pixels. For each pixel of these areas, the *entropy* is calculated, then for each area or row we will have an *entropy curve* which, when smoothed, has as *many local maxima as lanes and as many local minima as lane division lines plus one. For the purpose of testing*, several real traffic scenarios under different weather conditions with other moving objects were used. However, these background objects, not on the road, were filtered out. *Our algorithm,* compared to others based on trajectories of vehicles, shows the following *advantages*: (1) the lowest computational time for lane detection (only 32 s with a traffic flow of one vehicle/sec per-lane); (2) better results under high traffic flow with congestion and vehicle occlusion. Instead of detecting road markings, it forms lane-dividing lines. Here, the entropies of Shannon and Tsallis were used, but the entropy of Tsallis for a selected q of a finite set achieved the best results.

48. An Alternative Approach to Experimental Design under Covariate Drift

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The application of machine learning and advanced statistical tools to complex physics experiments, such as Magnetic Confinement Nuclear Fusion, can be problematic due the varying conditions of the systems to be studied. In particular, new experiments have to be planned in unexplored regions of the operational space. As a consequence, care must be taken because the input quantities used to train and test the performance of the tools are not necessarily sampled by the same probability distribution as in the final applications. The regressors cannot therefore be assumed to verify the i.i.d. (independent and identical distribution) hypothesis and learning has therefore to take place under conditions of covariate drift. This issue is particularly problematic in the design of future devices. In the present paper, a new data driven methodology is proposed to guide planning of experiments and to explore the operational space and optimise performance. The approach is not based on making "a priori" assumptions about the probability distribution of the new experiments but on the falsification of the existing models. The deployment of Symbolic Regression via Genetic Programming to the available data is used to identify a set of candidate models, using the approach of the Pareto Frontier. The confidence intervals for the predictions of such models are then used to find the best region of the parameter space for their falsification, where the next set of experiments can be more profitably carried out. The procedure is repeated until convergence on a satisfactory model. Extensive numerical tests and applications to the scaling laws in Tokamaks prove the viability of the proposed approach.

49. An Application of the Improved Multiscale Weight Permuation Entropy to Complex Quantification of the Crude Oil Market

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Entropy measures are extensively used to study complex properties in nonlinear systems. Weighted permutation entropy (WPE) can overcome the ignorance of the amplitude information of time series compared with PE and shows a distinctive ability to extract complex information from data having abrupt changes in magnitude. In our work, we propose an improved multiscale WPE (IMWPE) method by combination of WPE and an improved multi-scale algorithm. By analysis of white noise and 1/f noise, it is validated that the IMWPE method can increase the entropy estimation accuracy compared with the MWPE method. Then, the empirical IMWPE analysis of Brent and Daqing crude oil is performed on return series, volatility series with multiple exponents and EEMD-produced intrinsic mode functions (IMFs) which represent different frequency components of the return series. It is shown that Daqing crude oil has relatively less complex properties, implying that the Chinese oil market is less efficient than the Brent-represented international oil market. The volatility series exhibits reduced complex properties with the increase of the volatility exponent. Through EEMD decomposition, distinctive complexities of different frequency time series are discovered.

50. An Integrative Framework for Scientific Research Evaluation Using Information Theory and Nonparametric Efficiency Analysis

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The latest performance evaluation trends in the Research and Development sector show that advanced methodologies in econometrics and operations research have proved extremely useful and relevant in analyzing the efficiency of various types of activities, including scientific research. In this paper, we review the latest conceptual approaches, methodologies and research tools from a complex inter- and trans-disciplinary perspective. Advocating for the assessment of scientific research in a comprehensive manner, subscribed to the logics of a society based on knowledge and innovation, we propose an information theory-based framework for analyzing performance in scientific research. Our approach investigates the relevance and effectiveness of various entropy measures and weighted entropy measures for assessing the diversity and efficiency of scientific research and further relies on a methodological apparatus that includes a series of factors with essential roles in research evaluation. The paper also contributes to the development and application of the most recent nonparametric techniques of efficiency measurement, and performance and ranking assessment of scientific research units.

51. Applying Spectral Clustering Techniques to Analyze the Online Communities of TV Characters and Programs: A Case Study of the Spanish Public Television

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Online social networks are becoming one of the main communication channels between end-users and products/services in which users are continuously participating in and generating new contents (texts, images, videos, etc.), forming opinions and creating implicit communities on specific topics. This environment is generating huge amounts of data including both contents and interactions that can be used to analyze the impact of marketing strategies or, even more, to understand users' behavior. The analysis of online social networks can provide very interesting insights with different purposes.

In this context, the media sector (more specifically the TV sector) is facing different challenges to take advantage of this new environment and provide better contents adapted to specific communities making a mapping between the virtual and real audience. As an example, some questions are emerging: Would it be possible to select the best team to make a TV program? Who would be the best guest to have on an interview program? Given a topic, can we select the best TV presenter?

Existing media organizations have estimations of how many spectators they have through the TV but the reality is that the use of the TV is evolving to an interactive environment of tailored contents anywhere, anytime. TV analysts are looking for new solutions to understand the needs of the audience and to provide them the best contents.

This work presents the application of spectral clustering techniques to analyze the evolution and behavior of large networks and infers new knowledge. A platform has been designed and implemented to continuously gather and analyze data coming from online social networks. More specifically, large graphs of the social connections, interactions and contents are being generated and studied, applying complex network analysis to understand and infer the implicit communities that are built around the TV characters and programs.

52. Bending, Stretching, and Smiling: Entropic Homeomorphisms of the Faces of Finance

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Parker (2016, 2017, and 2018) utilized concepts from information theory to study the effects of entropy on the behavior of finance systems and variables of interest. From this analysis, a common entropic measure was derived that determines the structure and evolution of a wide variety of financial topologies. This information theoretic variable is defined as the ratio of the arrival and processing rates of information at financial markets (R/C). Changes in R/C have intuitive effects on the distribution of returns, the volatility surface, and the yield curve. As the level and variance of (R/C) evolves, so does the amount of uncertainty in each of the corresponding markets. By utilizing R/C—the simplistic but often unrealistic shapes from financial theory—the normal distribution of returns, constant volatility across option strikes and terms to expiration, and the upward sloping yield curve are transformed into the complex and evolving structures of financial reality. The central role of this ratio elucidates a previously unknown and important connection between the disparate branches of finance.

53. Boltzmann Entropy v/s Gibbs Entropy: An Information Theory Approach

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Entropy S is one of most fundamental concepts in Thermodynamics and Statistical Mechanics; however, there is more than one way to calculate it, it can be associated to any variable and the interpretation of the results is not free of surprises. After defining entropy by means of three different equations, the classical textbook by Huang [1] makes the following warning which illustrates this point: "In fact if these definitions were not equivalent, the validity of statistical mechanics would be in doubt". In the present paper, we apply, compare and discuss two ways of calculating S for two well-known systems: (a) The Ising model; (b) The Potts model in the discrete clock model approach.

On the other hand, mutability has recently been introduced as a way to measure the information content in any data chain [2,3]. We will show that mutability follows very closely the behavior of Boltzmann entropy, with some differences and even some advantages near phase transitions. Applications of mutability to fields as diverse as magnetic transitions, stock market behavior, seismic activity, wind energy production and blood pressure characterization will be mentioned.

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54. Consciousness as a Global Property of Brain Dynamic Activity

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We seek general principles of the structure of the cellular collective activity associated with conscious awareness. Can we obtain evidence for features of the optimal brain organization that allows for adequate processing of stimuli and that may guide the emergence of cognition and consciousness? Analyzing brain recordings in conscious and unconscious states, we initially followed the classic approach in physics when it comes to understanding collective behaviours of systems composed of a myriad of units: the assessment of the number of possible configurations (microstates) that the system can adopt, for which we use a global entropic measure associated with the number of connected brain regions. Having found maximal entropy in conscious states, we then inspected the microscopic nature of the configurations of connections using an adequate complexity measure, and found higher complexity in states characterized not only by conscious awareness but also by subconscious cognitive processing, such as sleep stages. Our observations indicate that conscious awareness is associated with maximal global (macroscopic) entropy and with the short time scale (microscopic) complexity of the configurations of connected brain networks in pathological unconscious states (seizures and coma), but the microscopic view captures the high complexity in physiological unconscious states (sleep) where there is information processing. As such, our results support the global nature of conscious awareness, as advocated by several theories of cognition. We thus hope that our studies represent preliminary steps to reveal aspects of the structure of cognition that leads to conscious awareness.

55. Detection Algorithm of Trapped Victims under Complex Debris with UWB Radar Based on the Entropy Method

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Ultrawideband (UWB) radar is widely used in the post-disaster victim search and rescue field because of its characteristics of non-contact and penetrability through non-metal materials compared with other methods. Though a series of successful experiments and field tests were reported, victim detection with UWB radar under complex collapsed buildings still faces difficulties based on the traditional detection algorithms because the multi-path effect can lead to the received electromagnetic signal reflected by the structure of the collapsed buildings having respiration-like properties. Consequently, the misdetection rate increases under this scenario. Entropy, a measure for the amount of information that would be needed to specify the system, can be used as a parameter indicating the presence of victims as the received electromagnetic signal reflected by the trapped victim will be more in order than that reflected only by the clutters because the respiration and heartbeat signals are quasi-periodic. To testify the efficiency of the proposed algorithm based on the entropy method under the scenario of complex debris, simulated and field experiments were carried out. The result shows that the proposed algorithm can increase the detection rate compared with a benchmark detection algorithm, which indicates that the entropy method is promising in the field of victim search and rescue with UWB radar.

56. Determination of the Irreversible Entropy Generation Rate in Mobile Phone Batteries

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Ageing occurs in real systems undergoing energy transformations. In the field of electrical and electronic systems, devices undergo power losses, which are partially devoted to their degradation. Entropy generation rate has been recently proposed as a suitable method to describe system ageing. In this contribution, we investigate battery ageing by monitoring entropy production during real time operation. To know battery health is of paramount importance in order to develop mobility based on electrical vehicles, and present available methods are not reliable enough. We monitored current, voltage and temperature for several months in different mobile phones. Recorded data was categorized according to three power consumption levels: rest, medium power and high power, where the phone was demanding low, medium and high power capabilities of the battery respectively, depending on the load needs. Electrical data was processed to obtain thermodynamic properties. First, it was necessary to implement a simple model to infer the open circuit voltage during the battery lifetime. Then, reversible entropy evolution and irreversible entropy production rates were inferred. Reversible entropy, which is related to electrochemical reaction, was obtained from rest category measurements and compared with classical TdS thermodynamics equations. Irreversible entropy production rate, which is related to heat dissipation and battery degradation, was obtained at medium and high power categories, in the framework of irreversible thermodynamics. Results show an increase of irreversible entropy production with battery ageing. Thus, irreversible entropy production becomes a promising indicator of batteries' (and other system's) ageing.

57. Entropic Effects in Hydrated Proteins

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It is well known that, at high temperature, proteins denature due to the dominance of the entropic term TS in the Gibbs free energy $G = H - TS$. Yet the entropy contribution coming from the solvent water plays a role that is fundamental even at lower T. It is widely accepted that the water contribution to the total Gibbs free energy of the system must be taken into account in order to understand the mechanisms behind cold and pressure denaturation of proteins [1]. In particular, water's ability to form hydrogen bonds due to its polarity introduces a considerable amount of complexity that significantly affects the total entropy of the system and gives rise to phenomena such as the hydrophobic effect. Here, we use Monte Carlo simulations of a coarse-grained model to study protein folding and the hydrophobic effect in explicit bulk water. We show that by taking into account how the presence of the protein changes the water properties at the interface, our model provides an accurate description of the hydrophobic effect and produces results that are compatible with the predicted existence of a close stability region in the temperature–pressure plane in which the protein is folded [2], a result that is relevant for our understanding of the folding–unfolding mechanism and for applications such as protein design [3].

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58. Entropic Equilibria Selection of Stationary Extrema in Finite Populations

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We propose the entropy of random Markov trajectories, originating and terminating at a state, as a measure of the stability of a state of a Markov process. These entropies can be computed in terms of the entropy rates and stationary distributions of Markov processes. We apply this definition of stability to local maxima and minima of the stationary distribution of the Moran process with mutation and show that variations in population size, mutation rate, and strength of selection all affect the stability of the stationary extrema.

59. Entropic Potentials Can Be Probed by Photons

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Tiny dimensional systems have a different stress–strain response than to bulky counterparts, because of an additional nanothermodynamic energy term in the total thermodynamic energy of the system. Contrary to stronger interactions, being independent of the system's size, weak interactions are strongly dependent on local morphological features, e.g., the presence of nanocavities, and constraints that might restrict molecular translational motions. A photonic mapping of a nanothermodynamic potential through surface strain might well reveal polar-entropic competition and thermodynamic energy flow. However, any experimental demonstration is difficult as sophisticated experimental approaches are required. In this work, by applying vacuum ultraviolet laser modification of surfaces at 157 nm (bio-polymers or inorganic surfaces), morphological changes and excessive cavitations, implies a major entropic variation of a matrix–analyte system, due to molecular trapping within the photon-induced nano-cavities. The surface-strained field allows the identification of thermodynamic state variations under well controllable conditions and, it maps polar-entropic fields during dynamic interactions. It is shown that the confinement of adsorbed molecules within photon-induced nano-voids in matrices, is the source of an entropic nanothermodynamic potential, proportional to the number of nano-voids.
Polar and entropic interactions on matrices are measured by using White Light Reflectance Spectrometry that monitors the relative strain (swelling/deswelling) of the matrix. The methodology allows the development of nanothermodynamic sensors that monitor polar-entropic completion and nanothermodynamic energy flow in the *pJ* energy scale for bio-applications.

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60. Entropy Generation Analysis of Laminar Flows of Water-Based Nanofluids in Horizontal Microtubes under Constant Heat Flux Condition

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During the last decade, second law analysis via entropy generation has become important in terms of entropygeneration minimization (EGM), thermal engineering systems design improvement, irreversibility, and energy saving.In this study, heat transfer and entropy generation characteristics of flows of multi-walled carbon nanotube-basednanofluids were investigated in horizontal microtubes with outer and inner diameters of ~1067 and ~889 µm, respectively. Carbon nanotubes (CNTs) with an outer diameter of 10–20 nm and length of 1–2 micron as non-sphericalnanoparticles were used for nanofluid preparation, and water was considered as the base fluid. The entropygeneration based on the experimental data, as a significant key in the thermal design system, was examined forCNTs/water nanofluids. The change in the entropy generation was only seen at low mass fractions (0.25 wt.% and 0.5 wt.%). Moreover, to gain more insight into the entropy generation of nanofluids based on the experimental data, afurther analysis was performed on Al_2O_3 and TiO_2 nanoparticles/water nanofluids from the experimental database ofthe previous study of the authors. The corresponding results disclosed a remarkable increase in the entropygeneration rate when Al_2O_3 and TiO_2 nanoparticles were added to the base fluid.

61. Entropy of Various Matrix Energies for Complex Networks

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Matrix energy is the sum of the absolute values of its eigenvalues. In the context of networks, several different energies have been proposed, depending on the particular form of the network matrix. Examples include the regular energy defined over the adjacency matrix, the Laplacian energy defined over the Laplacian of the network, or the Randić energy based on the so-called Randić matrix, in which each entry is the inverse of the square root of the product of node degrees, if the two nodes are adjacent.

The main problem with the above definition of network energy is the fact that it is hardly operational. Defined over the entire network matrix, the energy of that matrix is a single number trying to describe the network. In large complex networks, there can exist heterogeneous parts of the network with highly diversified topologies and properties, resulting in significant variation of local energy.

In this work, we diverge from the traditional approach of computer science, where entropy is understood in the light of Shannon's information theory. Instead, we use entropy in the physical sense, as the measure of the dispersion of energy, where energy is computed from various network-invariant matrix representations. We look at how the entropy of various network energies changes with the gradual change of network topology and we compare energies of node egocentric networks with other well-known node descriptors, such as in-degree, out-degree, betweenness, local clustering coefficient, eccentricity, Bonacich power, Katz centrality, and other indexes. We experiment with various models of complex networks (random network model of Erdos–Renyi, small-world network model of Watts and Strogatz, preferential attachment model of Albert–Barabasi, random network model of Waxman) and we observe the behavior of energies and their entropies as the hyper-parameters of network models change.

62. Entropy-Based Feature Extraction for Electromagnetic Discharges Classification in High-Voltage Power Generation

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This work exploits four entropy measures known as Sample, Permutation, Weighted Permutation, and Dispersion Entropy to extract relevant information from Electromagnetic Interference (EMI) discharge signals that are useful in fault diagnosis of High-Voltage (HV) equipment. Multi-class classification algorithms are used to distinguish between and classify various discharge sources such as Partial Discharges (PDs), exciter, arcing, micro sparking and random noise. The signals were measured and recorded on different sites followed by EMI expert's data analysis in order to identify and label the discharge source type contained within the signal. The classification was performed both within each site and across all sites. The system performs well for both cases with extremely high classification accuracy within each site. This work demonstrates the ability to extract relevant entropy-based features to EMI discharge sources from the time-resolved signals requiring minimal computation, making the system ideal for a potential application to online condition monitoring based on EMI.

63. Entropy-Based Functional Magnetic Resonance Imaging

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The most commonly utilized algorithms for detecting brain activation on functional magnetic resonance imaging (fMRI) analysis are hypothesis-driven methods represented by a general linear model where the temporal reference pattern for the signal of neuronal activation is assumed to be an on–off boxcar function convolved with a hemodynamic response kernel. Another class of algorithms is data-driven methods represented by independent component analysis (ICA). The most prominent feature of ICA is the fact that brain regions are automatically correlated. How to select the maps of physiological interest out of numerous statistically independent patterns, however, still remains to be addressed in each experiment. We propose here a totally new approach to fMRI design in which sample entropy (SampEn) of the signal time-series is compared among brain regions as well as between stimulus conditions. Results from fMRI experiments at a 7 Tesla system with flipping checkerboard stimulation demonstrate that activation in the primary visual cortex can be detected as a decrease in SampEn during the stimulation compared to that of the control condition where the subject kept looking at a small fixation mark displayed at the center of the field of vision. Cortical regions believed to represent visual processing were detected as voxels which have significantly lower SampEn values than other cortical areas. Lower SampEn was interpreted to reflect the reduced randomness of the fMRI time-series due to specific neuronal activities. The entropy-based approach presented here provides an intermediate solution between hypothesis-driven and data-driven fMRI analyses. The technique is applicable to a wide range of cognitive and connectivity studies.

64. Free Final Time Input Design Problem for Robust Entropy-Like System Parameter Estimation

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Input design is the process of designing an optimal input signal that is used for actuation of the system to extract maximum information about system dynamics. The novelty of this work is to design the free final time constraint input signal which is then used in the robust system identification process. The solution of the constrained optimal input design problem is based on minimization of the extra state variable representing the free final time scaling factor, formulated in the Bolza functional form, subject to the D-efficiency constraint as well as input energy constraint. The objective function used for parameter estimation provides robustness regarding outlying data and was inspired by definition of Gibbs entropy. An innovative contribution of this work is to use obtained free terminal time inputs to examine the economic aspects between the imposed constraints on the input signal design, and the experiment duration while undertaking a robust identification experiment. The numerical results of the Least Squares, and the Entropy-Like estimators for system parameter data validation where measurements include additive white noise are compared using ellipsoidal confidence regions.

65. Geometrical Control of Ionic Transport at the Nanoscale

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Entropic transport is a ubiquitous phenomenon in confined driven systems where par-ticles move in the presence of walls or obstacles. The coupling between thermodynamic gradients and the phase space availability to the dynamics has shown to trigger newnonlinear transport properties, as recently investigated [1]. One of the most appealing applications of these phenomena is the nanofluidic ionicrectifier [2]. Such a device can conduct ionic current in a preferential direction and in-hibit current in the opposite direction. This is of great interest from the point of view of nanotechnological applications because it opens up the possibility to efficiently con-trol ionic species and fluid flow without mechanical elements such as pumps or valves. Here, we address the study of ionic current rectification by means of the Fick–Jacobsapproach [3], a powerful mean field theory that treats the effect of geometrical con-finement as external entropic potential. We present a theoretical model for the response of a charged conical-shaped channel filled with a symmetric electrolyte. We derive analytical expressions for the fluxes in-side the channel and we define a quantitative measure of rectification efficiency. In particular, we investigate the dependence of rectification on the surface charge den-sity, the channel shape and the ionic strength of the reservoir. In contrast to the current understanding, we identify a regime where the rectifying behaviour of the system is driven by the surface conductivity ratio Dukhin parameter rather then the electrical double layer overlap.

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66. Heart Rate Variability Analysis Using Non-Additive Statistical Physics

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The state of the autonomic nervous system (ANS) may be monitored using heart rate variability (HRV) analysis. ANS regulation is a nonlinear, complex system with several delay control loops. Non-additive statistical physics has only been applied to this system in a limited way—to the HRV of a small number of healthy subjects.

Our aim is to present the results for SampEnq (a Tsallis entropy version of SampEn) applied to 24-h HRV recordings for 59 healthy individuals aged 20–70 y, in two sets of age, sex and disease control pairs for the risk of cardiac arrest and for the risk of death due to aortic valve replacement surgery. To obtain the appropriate Tsallis parameter q, SampEnq for the original data was subtracted from SampEnq for the random shuffled surrogate data. The parameter q_{max}, for which the difference *SDiffq* was the largest, was recorded. Calculations were performed both for 24-h data, for the nighttime parts and using sliding time windows of different lengths. A multiscale version of the method was also introduced.

It was found that *SDiffq* increases with the age of a healthy subject but q_{max} is practically independent of age, indicating unchanging properties of the empirical distribution of the data. The results for the two sets of control pairs are intriguing, e.g., no difference was found between members of pairs for cardiomyopathy while for coronary artery disease a definite pattern is visible for six of eight pairs. q_{max} defines the parameter value for the q-distribution. However, Tsallis defined the q-distributions as symmetric while empirical HRV distributions are mostly asymmetrical. The possibility of fitting an asymmetrical q-distribution to HRV data and its possible physiological interpretation will be discussed during the presentation.

67. Information Topological Characterization for Non-Stationary Random Processes

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To characterize the probability measure of a stochastic process, we study its associated dilation matrices. When the process is stationary, only a single dilation matrix describes the process' spectral measure: the well-known Naimark dilation. When the process is non-stationary, the dilation theory gives rise to a set of dilation matrices, which represent the spread of the spectral measure of the process. We focused in this work only on the subclass of real periodically-correlated processes. This leads to study only a finite set of real dilation matrices due to the periodicity. Finally, even though these matrices are theoretically of infinite dimension, we can truncate them in order to obtain rotation matrices, belonging in our case to the group SO(n).

This set is then analyzed as a data point cloud, which samples the space of all possible realizations of dilation matrices that can be drawn from the random process. To do this, we carry out a persistent homology calculation on this point cloud, where the metric between two points is given by the natural distance on SO(n). These calculations are summarized in a persistent diagram from which we assign a set of particular features in order to define the non-stationary and periodically-correlated process. Among those features, the so-called persistent entropy, which is a measure of the disorder of the diagram, plays a crucial role. We have then conducted a classification experiment by generating several random samples from different types of periodically-correlated processes, and we succeed in classifying them according to the persistent homology features of their dilation matrices. We finally claim that the principal components of the dilation matrices point cloud can be revealed by the persistent entropy features of the associated non-stationary process persistent diagram.

68. Information-Theoretical Space from Simple Atomic and Molecular Systems to Biological and Pharmacological Molecules

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In this work, we present an information-theoretical space generated from the Shannon entropy, the Fisher information, and the disequilibrium measures along with their corresponding Fisher–Shannon and LMC complexity measures. This unveils the unique physical, chemical and biological aspects of a great diversity of many-electron systems, ranging from neutral and ionized atomic systems and simple molecules to much more complex systems such as amino-acids and pharmacological molecular ensembles. This endeavour is achieved based on the theoretical ground that atoms and molecules can be described through the basic information-theoretical notions of delocalization, order, uniformity and complexity, thus revealing that a universal three-dimensional information-theoretical space for all systems of Nature might exist. The macroscopic atomic and molecular features are described by means of the entropy-like notions of spatial electronic delocalization, order, and uniformity. Hence, an information theory three-dimensional space (IT-3D) emerges that allows systems with common properties to be gathered

69. Irreversible Entropy Production in Fresh and Aged LithiumIon Cells

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Determining aging in lithium-ion batteries is very challenging because batteries are complex systems. They are composed of different elements, such as electrodes, current collectors, an electronic separator and the electrolyte, and each undergoes different degradation mechanisms. At present, degradation in lithium-ion batteries is commonly evaluated by indirect measurements, such as voltage or capacity, which do not provide a satisfactory aging characterization. Instead, we propose entropy, which is, by definition, directly related to the degradation itself, as an aging estimator candidate.

For that purpose, we have aged lithium-ion cells by cycling them at moderated charge/discharge rates at room temperature. We have evaluated the rate of irreversible entropy production in fresh and aged cells. Moreover, we have evaluated the entropy production by means of half-cells to discriminate the contribution to entropy of each electrode. Before the aging test, we found that the negative electrode was producing irreversible entropy faster than the positive one. However, the positive electrode suffered the highest increase in irreversible entropy production during the aging test. Thus, the positive electrode is the highest contributor to entropy generation at the aged state.

Furthermore, we have found a relationship between the phase transformations taking place during lithium insertion/extraction and the rate of irreversible entropy production. In particular, we have found that irreversible entropy is produced faster with each phase change, indicating that the degradation of the cells is mainly produced at the last stages of phase transformations.

70. Lithium-Ion Battery State of Health Analysis from Entropy Variations

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To obtain information on battery state such as the State-Of-Health (SOH), different techniques can be used, such as capacity measurement, impedance spectroscopy, internal resistance measurement, etc. However, few results are concerned with the use of the entropy-variations of a battery cell. This is mainly due to the fact that, as far as we know, no available methodology can quantitatively link SOH to entropy-variations. This study considers this issue. First, a testbed has been developed including different commercial battery cells, and experimental tests have been done. In particular, the cells have been cycled and entropy-variation profiles have been measured with the potentiometric method at different SOHs. Using machine learning techniques, we have then been able to quantitatively estimate SOH from entropy-variation profiles. The purpose of this study is to show that entropy-variation measurement can be an efficient way to acquire a better knowledge on battery state. It is a new step toward the safer use of batteries.

71. Macroscopic Entropy and Information of Non-Equilibrium Systems and New Formulation of Irreversible Thermodynamics. Application to Image Processing of Electron Microscopy of Sulfide Catalysts

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In this report, we consider the arbitrary changes of state of a non-equilibrium system, which can be isolated from the environment in each moment of time t. Isolating a non-equilibrium system tends to increase its entropy from $S(t)$ to the maximum entropy $S_o(t)$. The entropy increment is $I(t) = S_o(t) - S(t) \geq 0$. The entropies S and S_o relate to uncertainty in non-equilibrium and equilibrium systems, respectively. Consequently, the entropy increment relates to the information in a non-equilibrium system. Using equality $S = S_o - I$, we can write a new representation of the entropy differential dS in the form $dS = dS_o - dI$. Instead of the entropy production $d_iS/dt \geq 0$, we use dI/dt, where $I \geq 0$. Using dI/dt, we obtain accompanying formalism and new properties of a non-equilibrium system. For example, we can establish a general evolution criterion $d_X(dI/dt)/dt \geq 0$ (instead of the well-known Glansdorff–Prigogine criterion) which allows changes with time in the thermodynamic parameters at the boundary.
This relationship between entropy and information ($I = S_o - S$) was used for processing images of nickel–tungsten sulfide catalysts obtained by the method of high-resolution transmission electron microscopy. It was established that prepared catalysts consisted of plates (slabs) combined with thin nanolayers. The slab stacking degree distribution can be obtained from the image of sulfide catalysts. We showed that entropy and information obtained from this distribution according to the Shannon's formula are related to the preparation method. We discuss the relation between the properties of sulfide catalysts and entropy as well as information obtained from the images.

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72. Magnetic Entropy Changes in $La_{0.7}Ca_{0.3-x}Sn_xMnO_3$ ($0 \leq x \leq 0.1$) Compounds with a Second-Order Phase Transition

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In this work, we have investigated the magnetic entropy changes and MCE in $La_{0.7}Ca_{0.3-x}Sn_xMnO_3$ compounds which were prepared by a conventional solid-state reaction method. Three samples of $La_{0.7}Ca_{0.3-x}Sn_xMnO_3$ compounds were pressed into pellets at 200 °C. Magnetization measurements versus temperature revealed a decrease of the ferromagnetic–paramagnetic phase transition temperature (T_C) with increasing Sn-doping content. The T_C values are found to be 176, 171, and 164 K for x = 0.02, 0.04, 0.1 samples, respectively. Based on the magnetic field and temperature dependences of magnetization, we show these compounds undergoing a second-order magnetic phase transition. Additionally, the magnetic entropy change (ΔS_m) of samples under an applied magnetic field of 10 kOe was calculated by using the isothermal magnetization data. We have found the maximum magnetic entropy change ($|\Delta S_{max}|$) and full width at half maximum (δT_{FWHM}) of $\Delta S_m(T)$ curves for all the samples. These values are $|\Delta S_{max}|$ = 1.65, 1.27, and 1.24 J kg^{-1} K^{-1}, and δT_{FWHM} = 35.1, 42.9 and 46.1 K for x = 0.02, 0.04, 0.1 samples, respectively. The relative cooling power (RCP) values are thus about 56.4, 50.9, and 49.9 J kg^{-1} for x = 0.02, 0.04, 0.1 samples, respectively, which are comparable with the values of some magnetocaloric materials.

73. Magnetic Entropy Changes in $La_{0.7}Ca_{0.3}MnO_3$ Compounds with Different Pressure

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Temperature change of a magnetic material associated with an external magnetic field change in an adiabatic process is defined as the magnetocaloric effect (MCE). Recently, a large magnetic entropy change has been found and intensively studied in perovskite manganites, owing to the possibility to use these materials as active magnetic refrigerants in magnetic refrigeration technology. In this work, we have investigated the magnetic properties and MCE in $La_{0.7}Ca_{0.3}MnO_3$ compounds which were prepared by a conventional solid-state reaction method. Three samples of $La_{0.7}Ca_{0.3}MnO_3$ compounds with different pressure of p = 1, 3, and 5 GPa (named P1, P3, and P5, respectively). The magnetic measurements show that all the samples exhibited a ferromagnetic–paramagnetic (FM–PM) phase transition at Curie temperature (T_C), which decreased gradually with increasing P. The T_C values were found to be 278, 274, and 270 K for P1, P3, and P5 samples, respectively. Additionally, the magnetic entropy change (ΔS_m) of samples under an applied magnetic field of 10 kOe was calculated by using the isothermal magnetization data. We have found the maximum magnetic entropy change ($|\Delta S_{max}|$) and full width at half maximum (δT_{FWHM}) of $\Delta S_m(T)$ curves for all the samples. These values are $|\Delta S_{max}|$ = 1.2, 0.8, and 0.6 J kg^{-1} K^{-1}, and δT_{FWHM} = 44.7, 50.9 and 72.6 K for P1, P3, and P5 samples, respectively. The relative cooling power (RCP) values are thus about 56.4, 50.9, and 49.9 J kg^{-1} for P1, P3, and P5 samples, respectively.

74. Mathematical Properties of the Hypoentropy and Maximum Hypoentropy Principle

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Hypoentropy was introduced by Ferreri in 1980. It boasts the parameter λ and covers the part under the entropy. If we take the limit λ to infinity, the hypoentropy becomes the usual entropy. In 2014, we published our paper entitled, "On Some Properties of Tsallis Hypoentropies and Hypodivergences" in *Entropy, 2014, 16, 5377-5399.* There, we studied some mathematical properties of Tsallis hypoentropies and hypodivergences. Based on these results, in this presentation, we focus on the maximum hypoentropy principle without the Tsallis parameter. That is, our purpose is to find the probability distribution such that hypoentropy is maximized under some assumptions. Firstly, we impose the condition that total probability is equal to one, and the mean is constrained to constant. Then, we derive the probability distribution that maximizes the hypoentropy. The obtained probability distribution is the canonical form with the parameter of hypoentropy and it covers the usual canonical probability distribution in the limit of λ to infinity. Secondly, we will try to find the probability distribution that maximizes the hypoentropy under the assumption that probability is equal to one, and the mean and the variance are constrained to constant.

75. Mutual Information Links Structural and Dynamical Properties of a GlassForming Liquid

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Supercooled liquids avoiding crystallization show an exponential slowing down of the dynamics, eventually falling out of equilibrium. This final state, namely glass, is an extremely interesting state of matter, with the disordered molecular structure typical of liquids but behaving like a solid from a mechanical point of view.

A key issue of the glass transition is to determine the link between the slowing down of the liquid dynamics and its structural arrangement, such as the growth of characteristic length scales. Despite important contributions to the glass transition coming from the most disparate fields, ranging from statistical physics to geology and engineering, little effort has been made to date to investigate the glass transition with the powerful tools provided by the information theory.

We present an information theory-based approach to investigate the growth of characteristic length scales associated with the slowing down of the liquid dynamics, using coarse-grained Molecular Dynamics simulations of a fully-flexible polymer melt. Following similar findings on a system of hard spheres [1], we employ Mutual Information as a measure of general correlation between the displacement probabilities of pairs of particles, defined as a function of their Shannon Entropies. This approach allows to explore to what extent dynamics at a given time is encoded in the initial configuration. We observe a highly correlated cluster of particles of growing size at the characteristic time scale associated with the structural relaxation of the system.

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76. On Energy Transformation and Entropy Production in a DC Gas Discharge

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Physical plasma is a complex system which can serve for studying a multitude of phenomena and processes taking place outside the thermodynamic equilibrium. Close to equilibrium, a plasma system reacts to any external constraint, shielding any outer influence. In this way, the plasma system tends to preserve its thermal equilibrium, behaving as an asymptotically stable system. However, when the external constraint increases, the physical plasma adapts itself to the constraint, displaying strong nonlinear behaviors. One of the consequences of driving away from the thermodynamic equilibrium of a plasma (by continuously injecting matter and energy into the system) is the appearance of one or more balls of fire in front of the anode of the discharge tube. The ball of fire is a self-organized space charge structure confined by an electrical double layer that acts as an internally built source of particles and energy, being related to a negative differential resistance, which amplifies the current in the electrical circuit of the discharge. The formation of this ordered and coherent structure marks the transformation of part of the thermal, disordered energy of the electric charges into the electric potential energy of the structure, i.e., ordered energy. The non-equilibrium phase transition that takes place at the formation of a ball of fire minimizes the free energy of the system and represents the system's reaction to the external constraint.
The present contribution investigates the energy transformation during the evolution of the system and, also, the entropy variation during the dynamics presented above, which culminates with the self-assembling of the ball of fire in front of the anode of the DC gas discharge.

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77. On Normalized Mutual Information: Measure Derivations and Properties

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Starting with a new formulation for the mutual information (MI) between a pair of events, this paper derives alternative upper bounds and extends those to the case of two discrete random variables. Normalized mutual information (NMI) measures are then obtained from those bounds, emphasizing the use of least upper bounds. Conditional NMI measures are also derived for three different events and three different random variables. Since the MI formulation for a pair of events is always nonnegative, it can properly be extended to include weighted MI and NMI measures for pairs of events or for random variables that are analogous to the well-known weighted entropy. This weighted MI is generalized to the case of continuous random variables. Such weighted measures have the advantage over previously proposed measures of always being nonnegative. A simple transformation is derived for the NMI, such that the transformed measures have the value-validity property necessary for making various appropriate comparisons between values of those measures. A numerical example is provided.

78. Point Information Gain, Point Divergence Gain and Multidimensional Data Sequence Analysis

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We generalize the point information gain (PIG), the point divergence gain (PDG), and derived quantities, i.e., a point information gain entropy (PIE), a point information gain entropy density (PIED), a point divergence gain entropy (PDGE) and a point divergence gain entropy density (PDGED), which are derived from the Rényi entropy and describe spatio-temporal changes in discrete multidimensional distributions. The behaviour of PIG and PDG is simulated for typical distributions. PIG, PDG and related entropies overcome all existent approaches by the possibility to make provision for the local surroundings. The PIE/PIED spectrum may be used as a unique classifier of the dataset (i.e., image). PDG is a generalised subtraction which takes into account the distribution of datasets which are mutually subtracted. We further demonstrate the main properties of PIE/PIED and PDGE/PDGED spectra for the real data with the examples of several images and discuss further possible utilizations in other fields of data processing. The approach was successfully used in diverse fields such as superresolution microscopy, animal and human behaviour detection and human perception classification.

79. Predominant Information Quality Scheme for the Essential Amino Acids: An Information-Theoretical Analysis

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In this work, we undertake a pioneer information-theoretical analysis of 18 selected amino acids extracted from a natural protein, bacteriorhodopsin (1C3W). The conformational structures of each amino acid are analyzed by use of various quantum chemistry methodologies at high levels of theory: HF, M062X and CISD(Full). The Shannon entropy, Fisher information and disequilibrium are determined to grasp the spatial spreading features of delocalizability, order and uniformity of the optimized structures. These three entropic measures uniquely characterize all amino acids through a predominant information-theoretical quality scheme (PIQS), which gathers all hemical families by means of three major spreading features: delocalization, narrowness and uniformity. This scheme recognizes our major chemical families: aliphatic (delocalized), aromatic (delocalized), electro-attractive (narrowed) and tiny (uniform). All chemical families recognized by the existing energy-based classifications are embraced by this entropic scheme. Finally, novel chemical patterns are shown in the information planes associated with the PIQS entropic measures.

80. Probabilistic Approach for Image De-Noising

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Live cell and intra-vital microscopy imposes limitations on the intensity of sample illumination due to the photo-induced generation of reactive oxygen species and concomitant phototoxicity. The necessity to follow fast intracellular processes limits the single image exposure time. These two limitations result in a low signal-to-noise ratio (SNR) in the live cell and intra-vital microscopy images and makes them difficult to segment. Many de-noising algorithms have been developed to date. In essence, de-noising algorithms balance noise suppression and image blurring. For example, classical edge-preserving de-noising algorithms (e.g., median filtering, anisotropic diffusion) were developed to de-noise only a homogenous area, while limiting the blurring of the objects of interest. Unfortunately, the low contrast and diffraction-limited size of intracellular structures result in sub-optimal quality of de-noised images. More sophisticated state-of-the-art probabilistic algorithms such as PureDenoise [Blu and Luisier, 2007], PureLet [Luisier, 2010], CTV [Beck and Teboulle], and SRF [Haider, 2016] produce much better results. However, the problem of de-noising of low SNR fluorescent microscopy images is still a challenging one.

Previously, we proposed a probabilistic de-noising algorithm BFBD [Kalaidzidis, MaxEnt 2015] for low SNR fluorescent images. Unfortunately, the BFBD algorithm had two drawbacks: (1) the final probability estimation requires numerical integration; (2) estimated intensity depends on prior parameters which were assigned by end-user. In this work, we made two contributions: (1) found analytical expression for de-noised intensity estimation; (2) developed a "leave-one-out" approach, where the intensity fluctuations of all pixels of the image, but not the estimated one, were used to define prior parameters. A new de-noising algorithm was compared with classical (median filtering, Gauss low-pass filtering, anisotropic diffusion) and state-of-the-art (PureDenoise, PureLet, SRF) algorithms and demonstrated high-quality image de-noising.

81. Quantifying Link Predictability of Complex Networks

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From the promotion of social friendships to personalized recommendations of e-commerce even for identifying possible interactions in biological networks, the prediction of missing links underlies a wide range of practical applications. Although the link prediction problem has been studied extensively and a large number of prediction algorithms have been proposed, different algorithms usually provide different accuracies in the same network, yet there are different definitions of the accuracy itself. Thus, the intrinsic link predictability of a network still remains unknown. In other words, for a given network, we still do not know the best prediction accuracy achievable in the ideal case (an omniscient algorithm), which is a long-standing problem in network science. Here, we address this problem by studying the relationship between the link predictability and the network Kolmogorov complexity that quantifies the amount of information in networks. We find that such a relationship allows us to collapse the predictability of networks from different fields into a single curve, indicating that all networks tend to follow the same universal pattern. Based on the observed pattern, we further obtain the upper bound and lower bound of prediction accuracy achieved by an omniscient algorithm by solving corresponding optimization pr oblems. These results not only help us uncover basic mechanisms that govern the link prediction problem, but also offer reliable measures to evaluate the performances of prediction algorithms associated with the network.

82. Random Spacing between Metal Tree Electrodeposits in Linear DLA Arrays

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When we examine the random growth of trees along a linear alley in a rural area, we wonder what governs the location of those trees, and hence the distance between adjacent ones. The same question arises when we observe the growth of metal electro-deposition trees along a linear cathode in a rectangular film of solution. We carry out different sets of experiments wherein zinc trees are grown by electrolysis from a linear graphite cathode in a 2D film of zinc nitrate solution toward a thick zinc metal anode. We measure the distance between adjacent trees, calculate the average for each set, and correlate the latter with probability, fractal dimension and entropy. We also attempt to obtain a computational image of the grown trees as a function of parameters such as the cell size, number of particles and sticking probability. The dependence of average distance on concentration is studied and assessed.

83. Reconstructing Uncertain Graphs Based on Low-Rank Factorizations

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Recently, Uncertain Graphs (UGs) have been found to be a useful model in a plethora of applications, ranging from biological networks (e.g., protein–protein interaction networks) to social networks. In the related literature, there is a research effort towards adapting classical data analysis procedures from deterministic graphs to this new representation, including k-nearest neighbours, graph clustering and low-dimensional graph embeddings. Assuming that any edge can exist independently, the UG can be characterized by a multivariate Bernoulli distribution, and therefore the amount of uncertainty in a given UG can be measured by the average edge entropy. In this work, we study the problem of uncertainty reduction, which is described as follows. Given a UG, we want to derive a compressed representation UG = UG(θ), where θ is a set of parameters, so that UG resembles the original UG with reduced uncertainty. By parameterizing UG, some prior knowledge or assumption regarding the global graph structure can be incorporated, so that the feature learning task can be interpreted as a denoising process. We introduce a statistical model of UGs and we propose algorithms for uncertainty reduction based on non-linear optimization of an energy function E, similar to the notion of m-projection in information geometry. This uncertainty reduction methodology can serve as a general procedure for other learning tasks, e.g., classification or clustering a given set of UGs.

84. Reducing Cross Entropy to Not Cross Paths: Improving Multiagent Underwater Vehicle Coverage Planning

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We investigate the use of entropy-based methods to improve the performance of unmanned underwater vehicle (UUV) teams for large-scale geospatial tasks such as coverage planning. Major challenges to low cost long duration missions include expensive underwater positioning systems and energy storage for propulsion. It is advantageous to exploit the currents of the ocean to increase endurance. Forecast uncertainty must be accounted for, requiring the generation of feedback plans. Multiagent coverage planning for UUVs is an unresolved challenge because overlaps in coverage incur penalties, making techniques such as dynamic programming impractical given the size of the environment of interest. To tackle this challenge, we identify two state-of-the-art approaches, Monte Carlo Tree Search (MCTS) and Cross Entropy Method (CEM) and benchmark them against a default policy in an NCOM ocean simulation of the Gulf of Mexico. MCTS combines multi-armed bandit techniques with graph-based search to guide Monte Carlo roll-outs to greater rewards. On the other hand, CEM iteratively updates the parameters of the importance sampling density to minimize the cross entropy, which in turn increases the probability of detecting the optimal solution. After tuning algorithm parameters, we validate results planning for 10 agents in a 3 deg (~300 km) square over 100 deployment scenarios, showing that CEM improves the default policy by 39%, while MCTS improves the default policy by 29%. This implies that CEM generates plans that cover 6.9% more area than MCTS on average.

85. Relating Vertex and Global Graph Entropy in Randomly Generated Graphs

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Global measures of entropy capture the complexity of a graph, but rely upon the calculation of its independent sets, or collections of non-adjacent vertices. This decomposition of the vertex set is a known NP-Complete problem and for most real-world graphs is an inaccessible calculation. Recent work by Dehmer et al. and Tee et al., identified a number of alternative vertex level measures of entropy that do not suffer from this pathological computational complexity. In recent work, we demonstrated that the usage of these local measures in identifying important nodes in large-scale computer networks is very effective, and can also be used to build a model of scale-free networks. It is intriguing to consider whether the link between local and global entropy measures is more fundamental. In this paper, we investigate the existence of a correlation between vertex level and global measures of entropy, for a variety of randomly generated graphs. We use the greedy algorithm approximation for calculating the chromatic information and therefore Körner entropy. We are able to demonstrate a close correlation for this narrow subset of all graphs and outline how this may arise theoretically.

86. Relative Fisher Information of D-Dimensional Isotropic Harmonic Oscillators and the Morse Potential Systems

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The radial and angular structures of wave functions, derived as exact solutions of the Schroedinger equation for physical systems, provide a fundamental ingredient that links physics and the contained information. Entropy and Fisher information calculations of hydrogen-like atoms and other quantum systems have been extensively studied, which entails cumbersome integrations of orthogonal polynomials such as Hermite, Laguerre, Gegenbauser, etc. In this presentation, by setting the ground state as a reference density, we calculated the relative Fisher information of the two prototypical density functions: the radial density functions of the D-dimensional isotropic harmonic oscillators and the Morse potential systems. In the recent study, [T. Yamano, Chem. Phys. Lett. **691** (2018) 196], the author reported that the relative Fisher information for hydrogen-like atoms decreases with the principal quantum number by specifying 1 s orbital as a reference state. Since the exact wavefunctions for these systems contain the associated Laguerre polynomials, this study provides an interesting comparison with the results for the hydrogen-like atoms.

87. Strong Entropic and Electric Current Coupling and Surface Topology in 2D Semiconductors Violates Translational Current Homogeneity along Opposite Conductive Paths at the Nanoscale

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The topology of amorphous or crystalline 2D semiconductors at the nanoscale implies a diversity of kinetic and electrical characteristics, and even then, there is a huge variation in the physical properties of the same material structure. Some of the different properties, including variable conductivity, current, and thermal instabilities, were generally understood on the basis of electron grouping between the interface of nanodomains and the different size of localized electron energy levels where translational symmetry and current homogeneity along opposite directions were retained.

In this work from the scanning force, thermal, conductive and electrical microscopy analysis in amorphous semiconductors, it was shown that at the nanoscale the surface topology of 2D semi-conductive materials regulated different current flow stability along opposite conductive directions and 2D topology was also closely connected with both thermal and electric properties as a result of strong entropic and electric current coupling.

It was also evident from the experimental results and within a theoretical framework that for long conductive paths (>1 μm), current flow exhibited bidirectional stability. On the contrary, at the nanoscale and for short conductive paths, there was only unidirectional current stability. The 2D translational degeneracy of current flow along opposite conductive paths at the macroscopic level was raised by the strong electric and entropic current coupling that either amplified or dumped the current fluctuations for antiparallel directions [1].

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88. Synthetic Graphical Analysis of the Thermoelectric Systems Operating Modes

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The original representation of bithermal systems in the normed ternary diagram (Qh, Qc, W) allows a synthetic graphical analysis of the operating conditions attainable. Depending on the energy flow directions, four distinct operating modes, distributed into sectors of angle pi/3, are identified: two potentially reversible operating modes (heat engine and heat pump) and two dissipative operating modes (forced heat transfer and thermal dissipation). The second law of thermodynamics restricts the possible operating conditions to the top half-plane bounded by the Carnot boundary limit (straight line passing through the origin whose slope is a function of the sources temperature). Using polar coordinates allows an intuitive graphical interpretation: the energy flow intensity involved in the system is linked to its distance to the origin and its efficiency is only related to the angle alpha from the normal to the axis Qh. The entropy generation is thus graphically deduced from the angular difference between the operating point and the Carnot boundary limit.

Based on the standard model of Ioffe, the operating conditions of thermoelectric systems are plotted in the proposed representation as a parametric curve function of the electrical intensity (for given temperature sources). This way, the specific contributions of each phenomenon involved in the semiconductor are discussed in terms of entropy generation: reversible Seebeck effect, irreversible heat leakage by conduction and irreversible thermal dissipation by the Joule effect. The threshold of each operating mode, along with the efficiency and powers of the heat pump and heat engine modes, are characterized graphically and analytically as a function of the material properties and the operating conditions. The influence of the electrical intensity on the targeted operating conditions (maximum efficiency vs. maximum power) is thus highlighted. Finally, the impact of the exo-irreversibilities on the operating conditions is analyzed with the introduction of external thermal resistances.

89. The Application of the Maximum Entropy Method for Improving the Efficiency of the Ultrasonic NDT

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Developing reflectors image reconstruction methods of both high-resolution and low-level of noise will allow the flaws to be more reliably detected and their sizes to be determined, thus improving the effectiveness of ultrasonic non-destructive testing. The nonlinear imaging methods should improve the NDT quality. There are several examples of the maximum entropy method (MEM) application for processing the ultrasonic echoes in order to restore the reflectors image at both beyond Rayleigh limit super-resolution and high SNR considered in the article. The use of a complex Barker code phase-manipulated signal as a transmitted pulse, along with compression by the MEM, the echoes measured by a single element transducer made it possible to increase—in a model experiment—the SNR of the image of a flat-bottom hole of 1 mm in diameter by more than 20 dB. Using a modification of the MEM is considered for restoring the TOFD-image, taking into account the signal shape measurement dependent on the depth of reflector occurrence.

The MEM can be used for processing echo signals measured by antenna array. The 2.5D-images of the crack models have been received, allowing their size to be specified. In the model experiment, while restoring the image of the reflector by the MEM in an object with structural noise, the SNR increased by more than 12 dB. In order to speed up the registration of echoes in the FMC mode, it was proposed to use CDMA technology based on simultaneous emission of pseudo-orthogonal signals by all elements of the array. The numerical experiment evidenced the effectiveness of applying the MEM both for decoding echo signals and for direct reconstruction of the reflectors image by the MEM based on the sum of the echoes. A set of model experiments showed the effectiveness of the MEM for obtaining reflectors images at super-resolution and at a low level of noise.

90. Application of the Entropy Principle to Solve the Tomographic Problems in Physics and Medicine

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The entropy concept is known as a powerful method for solving various classes of ill-posed inversion problems, including the reconstruction tomography. A review of the applications of the entropy principle in solving tomographic reconstruction problems in plasma physics, physics of flames and nuclear medicine is presented in this paper. The studied plasma objects were different in their parameters. For instance, a microplasma of 0.05 cm and methane plasma in a plasma-chemical reactor of 40 cm, the plasma of light sources with mercury pressure of 3 atm and capillary light sources with gas pressure of 0.001 atm were studied. Stationary and temporal tomographic reconstructions are considered in the review. A specific difficulty of flame tomography is the character of the source function to be reconstructed: the function describing the reaction zones has narrow high-gradient peaks. The entropy-based reconstruction method combined with the local regularization of the data pre-processing procedure was developed to achieve more accurate reconstruction of the peak intensities and was applied for the reconstruction of reaction zones in the propane-air flame of a Bunsen-type burner. The entropy concept was also used in reconstruction of images by single photon emission computed tomography (SPECT) in nuclear cardiology. The entropy-based maximum a posteriori (MAP) reconstruction method was evaluated for its efficacy in the myocardial defect reconstructions. The results of simulations have shown that this method is a promising approach in SPECT imaging.

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92. Thomas Jefferson, John Quincy Adams, Jeremy Bentham, and John Nash—Optimal Integer Solution of α-Divergence for the Apportionment of Representatives Problem

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"One-vote one-value" is a core principle of equality. The quotient of representatives (n_j/n) should be equal to the quotient of the population (N_j/N); however, it is almost impossible.

Many politicians and mathematicians insist on using divisor methods, wherein they find a divisor d such that the values of n_j's (which are the special rounded numbers of the quotients of states N_j/d) add up to n. Here, special rounded means rounded up when the quotient is equal to or bigger than "a mean." Thomas Jefferson insisted on using maximum (n_j) for the thresholds, and John Quincy Adams insisted on using the minimum ($n_j - 1$). Huntington (1928), who was the president of the Mathematical Association of America, recommended using the geometric mean ($\{(n_j - 1)n_j\}^{1/2}$) or Hill's method. This method was employed by the US House; however, there is still strong support for using arithmetic mean ($\{(n_j - 1) + n_j\}/2$) or Webster's method by Balinski-Young (1982).

Wada (2010, 2012) found that the aforementioned methods are obtained by maximizing the Kolm–Atkinson social welfare function or by minimizing the generalized entropy function which is parameterized by α ($\alpha \to \infty$: Jefferson, $\alpha = 2$: Webster, $\alpha = -1$: Hill, $\alpha \to -\infty$: Adams). Wada found that two more intuitive methods were supported by the Benthamian swf or Theil index ($\alpha \to 1$) and Nash swf or mld ($\alpha \to 0$) and recommended ($\alpha \to 0$). Wada (2016) generalized this idea using α-divergence which denotes the general utility function behind the veil of ignorance (uncertainty) and recommended using Kullback–Leibler divergence ($\alpha \to 0$).

93. Feeding Control and Microbial Cultivation Planning based on Relative Entropy

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Theoretical aspects for practical adaptive control applications that operate in unknown, nonlinear and time-varying biotechnological environments are still to be properly developed and implemented. Due to historic, reproducibility and restrictions imposed by regulations open-loop control approaches dominate in industrial fermentation processes. The scope of industrial challenges, when dealing with adaptive control, consist of, but are not limited to, sufficient modeling methods, the lack of state variables estimation tools or reliability of the sensors.
In this paper, we present a generic bioprocess grey box modeling approach that uses Maximum relative Entropy (MrE) to derive an optimization criterion to plan and/or predict the feeding solution profile. Our proposed design procedure has benefits for both existing industrial feed-forward and adaptive feedback control systems. To find grey box model's parameters, both control scenarios use MrE to introduce the cumulative glucose volume as uncertainty into convex optimization task. In the scenario of regular open loop biotechnological system, to evaluate the specific growth rate profile, one performs initial batch-type fermentation. The volume of the substrate fed during batch steps and observations of glucose concentration in the bioreactor media all help to evaluate the feeding solution (e.g,. glucose) consumption. After we identify grey box model's parameters through MrE, we describe the procedures to perform industrial limited growth processes by different limitation options and alternatives. Glucose concentration measurements are not necessary during those subsequent fermentations to identify the best run profile, which maximizes the desired property, e.g., maximum volume of a production property. In the adaptive control system though, our approach serves as a short-term forecast tool with which we are able to plan the substrate feed rate in online mode or could even evaluate the time moment of induction in the case of recombinant *Escherichia coli* microbial cultivation.

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