Book of Abstracts
40th International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering

Wolfgang von der Linden, Sascha Ranftl and MaxEnt Contributors

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Welcome Address

Dear long-time companions and dear newcomers to the realm of Bayesian inference, "the logic of science" as E.T. Jaynes put it. Welcome to the 40-th International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering!

It seems like yesterday that the series was initiated by Myron Tribus and Edwin T. Jaynes and organised for the first time by C.Ray Smith and Walter T. Grandy in 1981 at the University in Wyoming. Since then, tremendous progress has been made and the number of publications based on Bayesian methods is impressive. Despite the Corona pandemic, the 40th anniversary can finally happen, albeit a year late and only digitally. Nevertheless, we will have ample opportunity for reviews on the successes of the last four decades and for extensive discussions on the latest developments in Bayesian inference.

In agreement with the general framework of the annual workshop, and due to the broad applicability of Bayesian inference, the presentations will cover many research areas, such as physics (plasma physics, astro-physics, statistical mechanics, foundations of quantum mechanics), geodesy, biology, medicine, econometrics, hydrology, measure theory, image reconstruction, communication theory, computational engineering, machine learning, and, quite timely, epidemiology.

We hope you will enjoy the show

Wolfgang von der Linden and Sascha Ranftl
(Graz University of Technology, 2021)

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Special guests

40 Years of MaxEnt: Reminiscences

John Skilling
Maximum Entropy Data Consultants, Kenmare, Ireland.

Boltzmann's Life and Legacy: The Tragic Fate of a Great Scientist

Heinz Krenn
Institute of Physics, Karl-Franzens-Universität Graz, Austria.

Experimental Show: Entropy in Action

Gernot Pottlacher
Institute of Experimental Physics, Graz University of Technology, Austria.

Invited Talks

Tutorial: The Polya distribution or 'How many enrichment sites are there?'

Udo von Toussaint

Max-Planck-Institut for Plasmaphysics, Germany.

This tutorial illustrates Bayesian inference for Polya distributions. Polya distributions are important in many applications, e.g. recommendation systems or automated document classification approaches but do not belong to the exponential family. Exact and approximate inference is introduced using a fictitious example about the data based evidence of the existence of more than one enrichment site.

Key Words: Polya distribution, Exponential family, classification

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Tutorial: Inverse problems, Regularization and Bayesian Inversion and Machine Learning tools

Ali Mohammad-Djafari

ISCT, France.

This tutorial will introduce to traditional problems such as inverse problems, regularization methods, Bayesian inference or hierarchical prior models, and their solution with modern Machine Learning approaches such as Convolutional Neural Nets (CNN), Deep Learning and Physics-Informed Neural Networks (PINN).

Key Words: inverse problems, regularization methods, Bayesian inference, hierarchical prior models, machine learning, convolutional neural nets, physics-informed neural nets

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Inferring Change Points in the Spread of COVID-19 for Short-Term Forecasts

Johannes Zierenberg
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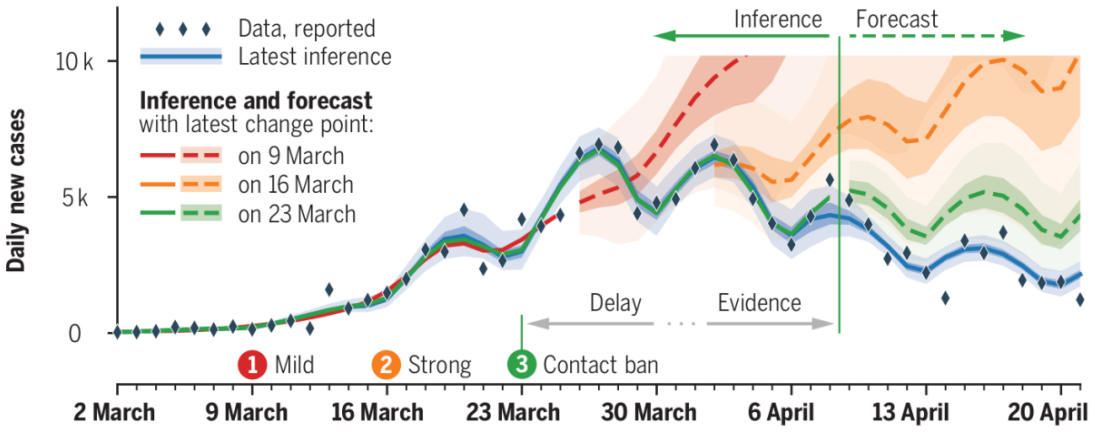
During the initial outbreak of an epidemic, reliable short-term forecasts are key to estimate medical requirements and capacities and to inform and advise the public and decision makers. In this initial phase, however, there is typically only little scientific knowledge about the disease such that relevant epidemiological parameters necessary for model forecasts need to be estimated from the little data available. In addition, key epidemiological parameters change over time when the society adapts to imminent dangers of an epidemic. In order to infer such (time-varying) epidemiological parameters for short-term forecasts, it is thus crucial to combine the available data with existing knowledge, a task perfectly suited for Bayesian inference. I will present such a Bayesian approach applied to inferring change points in the spread of COVID-19 [1] and discuss how this and similar approaches [2,3] can be a useful tool to assist decision making if the underlying assumptions and limitations are clearly communicated [4].

References:
[1] J. Dehning, et al., Science 369, 160 (2020).
[2] S. Flaxman, et al., Nature 584, 7820 (2020).
[3] J. M. Brauner et al., Science 371, 802 (2021).
[4] K. Soltesz, et al., Nature 588, 7839 (2020).



Quantum Mechanics as a Hamilton-Killing Flow on a Statistical Manifold

Ariel Caticha

Department of Physics, University at Albany – SUNY, USA.

The symplectic and metric structures inherent to Quantum Mechanics (QM) have been discovered, independently rediscovered, and extensively studied by many authors. Rather than postulating the Hilbert space structure of QM as a starting point, in this work we proceed in the opposite direction. Our goal is to derive or "reconstruct" the mathematical formalism of QM from more basic considerations of probability theory and information geometry. Our starting point is the recognition that probabilities are central to QM – they are not just a feature that is peculiar to quantum measurements. We derive QM as a particular form of entropic dynamics on a statistical manifold. For simplicity, here we restrict ourselves to the finite dimensional of a simplex. The important ingredients are two: on one hand the cotangent bundle associated to the simplex has a natural symplectic structure; and on the other hand, the cotangent bundle inherits its own natural metric structure from the information geometry of the underlying simplex. We impose a dynamics the preserves (in the sense of vanishing Lie derivatives) both the symplectic structure (a Hamilton flow) and the metric structure (a Killing flow). The result is a formalism in which the linearity of the Schrödinger equation, the emergence of a complex structure, Hilbert spaces, and the Born rule, are derived rather than postulated.

Model inversion in epilepsy for personalized medicine

Viktor Jirsa

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Over the past decade we have demonstrated that the fusion of subject-specific structural information of the human brain with mathematical dynamic models allows building biologically realistic brain network models, which have a predictive value, beyond the explanatory power of each approach independently. The network nodes hold neural population models, which are derived using mean field techniques from statistical physics expressing ensemble activity via collective variables. Our hybrid approach fuses data driven with forward-modeling-based techniques and has been successfully applied to explain healthy brain function and clinical translation including aging, stroke and epilepsy. Here we illustrate the workflow along the example of epilepsy: we reconstruct personalized connectivity matrices of human epileptic patients using Diffusion Tensor weighted Imaging (DTI). Subsets of brain regions generating seizures in patients with refractory partial epilepsy are referred to as the epileptogenic zone (EZ). During a seizure, paroxysmal activity is not restricted to the EZ, but may recruit other healthy brain regions and propagate activity through large brain networks. The identification of the EZ is crucial for the success of neurosurgery and presents one of the historically difficult questions in clinical neuroscience. The application of latest techniques in Bayesian inference and model inversion, in particular Hamiltonian Monte Carlo, allows the estimation of the EZ, including estimates of confidence and diagnostics of performance of the inference. The example of epilepsy nicely underwrites the predictive value of personalized large-scale brain network models. The workflow of end-to-end modeling is an integral part of the European neuroinformatics platform EBRAINS and enables neuroscientists worldwide to build and estimate personalized virtual brains.

Symmetries and Quantification: Why Mathematics Applies to the Real World

Kevin H. Knuth
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Many of us have a tendency to think of the laws of physics as mathematical laws dictated by Nature. But this raises serious questions as to why these laws and not others? How are such laws enforced and can they be broken? And why should these laws be mathematical in nature? More recently, some have proposed that universes form with random laws and that we could only have existed in a universe that happened to have the laws that we observe. But then one still wonders what are physical laws such that they can be "selected" at random? And why do they appear to be mutually consistent? And how are they enforced? Thinking about these questions, one cannot help but think that these ideas about physical laws are naïve at best. Richard Cox's foundation of probability theory provides a powerful clue in that it is clear that the laws of inference, the sum and product rules of probability theory, were determined by our desire to quantify degrees of logical implication using an ordered set of numbers and constrained by the fundamental symmetries of associativity and distributivity. One cannot help but wonder whether this situation is limited to probability theory, especially since the sum rule appears in multiple contexts across mathematics and physics. We argue that some of the laws of physics arise from the fact that we desire to simplify by describing things (or properties of things) with single attributes. It then happens that the symmetries force such description to be *isomorphic to* numbers with their sum and product rules. The result is a set of constraint equations that dictate how numbers are consistently assigned to quantify physical phenomena. These constraint equations are what we generally think of as the physical laws, while it is the underlying symmetries that form the foundation of Nature. These symmetries enforce the laws through constraint and ensure overall consistency. As a result, Mathematics, the human activity of assigning numbers to things in a manner that is consistent with the applicable symmetries, applies to the natural world.

* Kevin Knuth is grateful for the many years of friendship, collaboration, and influence of

The ABC of Physics

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Our description of objects is intrinsically and necessarily based upon observations derived from interactions. Classical macroscopic objects can remain unaffected by observation, but in the quantum domain, tiny objects will necessarily be perturbed by interaction. Here, we abstract this fact into an elementary assertion that quantity is inseparable from uncertainty. Unless the world is infinitely divisible, total precision must be unattainable. Uncertainty cannot be eliminated. Science's standard use of commonplace scalar arithmetic (the sum and product rules with their consequent mathematical superstructure) is justified by the basic symmetries of associativity and distributivity which apply to our descriptions of basic objects. In the context of a pair-valued fusion of quantity with uncertainty, those same basic symmetries yield the standard component-wise sum rule together with three allowed product rules. We call them A,B,C. The richness of the formalism of physics derives from that subtlety. For single objects, product rule A defines complex numbers, related to scalar observation through the probabilistic Born rule. This is why quantum theory is complex. For objects with properties, product rule B defines the Pauli matrices. There, we recognise first spin, and then energy-momentum as a 4-vector with Minkowski metric. Product rule C acts as an integrator, promoting energy and momentum to time and space. This is why we have three dimensions of space and one of time. Spacetime isn't a primary canvas onto which physics is painted. Although a critical tool in our descriptions and deeply embedded in our sensory intuition, relativistic spacetime is itself a quantum construct and part of physics. From this elementary foundation of quantity fused with uncertainty, we have derived the basic framework of physics, not through complication but through abstraction to deep simplicity. And of course the framework is self-consistent. Accept quantum formalism and the Schrödinger equation and the standard quantum commutation relations are immediate consequences, with the Heisenberg uncertainty relationships recovering the original assumption

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The Bayesian (r)evolution in the search for gravitational waves (a personal view)

Reinhard Prix

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When I entered the field of gravitational-wave data analysis about 15 years ago, the predominant probability paradigm in the community was still thoroughly Frequentist, with only a couple of Bayesian "rebel outposts". Since then things have changed in various interesting ways: by 2016 the paper on the first observation of gravitational waves used a hybrid of Frequentist detection- and Bayesian inference methods. This is still fairly typical: parameter-estimation inference is fully Bayesian, while the community employs a creative mix of a variety of methods and approaches for the initial search step of the data for candidates to follow-up. The relationship and interplay of "classical" statistical tools and the Bayesian framework for the detection problem is fascinating and surprisingly fruitful. In this talk I want to give a (personal) view of these developments and discuss a few key insights and applications from the field of gravitational-wave searches.

Sparse Stochastic Processes and the Resolution of Inverse Problems

Michaël Unser

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In this talk, we first present continuous-domain stochastic signal models that are compatible with the notion of sparsity. Specifically, we consider stochastic processes that are solutions of linear stochastic differential equations driven by white Lévy noises and we show that the non-Gaussian members of this family of processes admit a sparse representation in wavelet-like bases. We then apply our continuous-domain models to the discretization of ill-conditioned linear inverse problems where both the statistical and physical measurement models are projected onto a linear reconstruction space. We derive a class of maximum a posteriori (MAP) estimators which includes the popular Tikhonov and total-variation regularization schemes as special cases. We also develop efficient Gibbs sampling based algorithms to compute the minimum mean square error (MMSE) estimators which serve as our goldstandard. Finally, we apply our statistical framework to benchmark the performance of convolutional neural networks (CNNs) for deconvolution and Fourier sampling problems.

*Joint work with Pakshal Bohra.

Information field theory: from astronomical imaging to artificial intelligence

Torsten Enßlin

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Turning the raw data of an instrument into high-fidelity pictures of the Universe is a central theme in astronomy. Information field theory (IFT) describes probabilistic image reconstruction from incomplete and noisy data exploiting all available information. It uses methods from quantum field theory and statistical mechanics to construct optimal imaging algorithms. Astronomical applications of IFT are galactic tomography, gamma- and radio- astronomical imaging, and the analysis of cosmic microwave background data. This talk introduces into the basic ideas of IFT, highlights its astronomical applications, and explains its relation with contemporary artificial intelligence.

Uncertainty-Aware Numerical Solutions of ODEs by Bayesian Filtering

Hans Kersting
INRIA Paris & Ecole Normale Supérieure (ENS), France.

Numerical approximations can be regarded as statistical inference, if one interprets the solution of the numerical problem as a parameter in a statistical model whose likelihood links it to the information ('data') available from evaluating functions. This view is advocated by the field of Probabilistic Numerics and has already yielded two successes: Bayesian Optimization and Bayesian Quadrature. In an analogous manner, we construct a Bayesian probabilistic-numerical method for ODEs. To this end, we construct a probabilistic state space model for ODEs which enables us to borrow the machinery of Bayesian filtering. This unlocks the application of all Bayesian filters from signal processing to ODEs, which we name ODE filters. We theoretically analyse the convergence rates of the most elementary one, the Kalman ODE filter and discuss its uncertainty quantification. Lastly, we demonstrate how employing these ODE filters as forward simulators engenders new ODE inverse problem solvers tha t outperform its classical 'likelihood-free' counterparts.

Contributed Talks

Efficiency and cost optimization in surveys via haphazard sampling

M.G.R. Miguel, R.P. Waissman, M.S. Lauretto, J.M. Stern
University of Sao Paulo, Brazil.

Exploratory surveys with face-to-face interviews based on random or stratified sampling usually demand high sample sizes, and therefore, high infrastructure and staff costs. Even then, these experiments do not guarantee control of specific covariates, and may yield wrong inferences about parameters of the model. Our research group [1,2] has proposed the Haphazard Intentional Sampling Method, an allocation procedure that combines goal optimization techniques with random perturbations. The weight of the random perturbation can be calibrated in such a way that, on one hand, it is small enough to provide good representative samples and, on the other hand, it is large enough to break confounding effects and to avoid biased choices. In previous works, we compared the Haphazard Method with the Rerandomization method proposed by Morgan and Rubin [3] in benchmark allocation problems, and showed that the Haphazard Method provides allocation groups with a better balance and consistently more powerful inferences. In this work, we discuss advantages of the Haphazard Method in the context of census sampling, where the inference goal is to provide interval estimates for parameters of interest. We introduce a case study to estimate SARS-CoV-2 prevalence in main municipalities in Brazil. In comparison with rerandomization and single random allocation, samples yielded by the Haphazard method provide smaller and more consistent interval estimates for a given sample size. Interval size is the official goal set for studying the evolution of COVID-19 infection prevalence in Brasil. Therefore, the use of Haphazard Sampling has a great potential to contribute in the efforts to measure and control the spread of COVID-19 pandemy in Brazil.

References:
[1] M.Lauretto, R.Stern, K.Morgan, M.Clark, J.Stern (2017). Haphazard Intentional Allocation and Rerandomization. AIP Conf Proc, 1853, 05003, 1-8
[2] M.Lauretto, R.Stern, C.Ribeiro, J.Stern (2019). Haphazard Intentional Sampling Techniques in Network Design of Monitoring Stations. Proceedings, 33, 12, 1-9.
[3] K.Morgan, D.Rubin (2012). Rerandomization to improve covariate balance in experiments. Ann Statistics, 40, 2, 1263-1282
[4] Federal University of Pelotas. Evolucao da Prevalencia de infec¸cao por COVID-19 no Brasil: Estudo de Base Populacional. Technical Report (2020)

Key Words: Survey sampling, Haphazard allocation, Covid-19, SARS-CoV-2

Multi-level Markov chain Monte Carlo with maximally coupled proposals

Juan Pablo Madrigal Cianci and Fabio Nobile

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In this work we present a novel class of Multi-Level Markov chain Monte Carlo (ML-MCMC) algorithms based on maximally coupled [1] proposals, and apply them in the context of Bayesian inverse problems. In this context, the likelihood function involves a complex differential model, which is then approximated on a sequence of increasingly accurate discretizations. The key point of this algorithm is to construct highly coupled Markov chains together with the standard Multi-level Monte Carlo argument to obtain a better cost-tolerance complexity than a single level MCMC algorithm [2]. Our approach generates these highly coupled chains by sampling from a maximal coupling of the proposals for each marginal Markov chain. By doing this, we are allowed to create novel ML-MCMC methods for which, contrary to previously used models, the proposals at each iteration can depend on the current state of this chain, while at the same time, creating chains that are highly correlated. The presented method is tested on an array of academic examples which evidence how our extended ML-MCMC method is robust when targeting some pathological posteriors, for which some of the previously proposed ML-MCMC algorithms fail.

References:
[1] Torgny Lindvall. Lectures on the coupling method. Courier Corporation, 2002
[2] Tim J Dodwell, Chris Ketelsen, Robert Scheichl, and Aretha L Teckentrup. A hierarchical multilevel Markov Chain Monte Carlo algorithm with applications to uncertainty quantification in subsurface flow. SIAM/ASA Journal on Uncertainty Quantification, 3(1):1075–1108, 2015.

Key Words: Multi-level Methods, MCMC, Bayesian inverse problems

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Random Walk on simplex: Dirichlet distribution revisited

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The Dirichlet and the Dirichlet-multinomial distributions are of central importance in Bayesian inference as multivariate extensions of the beta and beta-binomial distribution. At the same time the Dirichlet distribution is the conjugate prior distribution of the multinomial distribution. In addition the Dirichlet distribution is suited as prior for discrete probability distributions, i.e. n-dim probability vectors confined to a unit n-simplex. For these reasons the Dirichlet distribution is ubiquitously used in many applications, ranging from clustering to document classification, further aided by the fact that independent multivariate Dirichlet distributed random samples can be generated efficiently [1]. However, - and perhaps surprisingly - there appears to be some confusion (c.f. [2-5]) about how to generate random walks on the n-simplex, which in some situations may be more efficient for inference tasks than the direct sampling approaches. Here we provide a suitable algorithm and apply it to a tracking problem.

References:
[1]L. Devroye, Non-Uniform Random Variate Generation, Springer (1986)
[2] J. Kokkala, https://stats.stackexchange.com/questions/103105/simplex-randomwalk (2014)
[3] P.C. Marques, https://stats.stackexchange.com/questions/103715/simplexrandom-walk-mean (2014)
[4] https://stats.stackexchange.com/questions/302502/how-to-implement-a-uniformrandom-walk-on-a-simplex (2017)
[5] https://en.wikipedia.org/wiki/User3aSkinnerd/Simplex Point Picking (2011)

Key Words: Dirichlet distribution, Random walk, Simplex

Legendre transformation for the maximum entropy theory of ecology

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One of the scientific fields in which the method of maximum entropy (MaxEnt) has been successfully applied is macroecology. The work of Harte and collaborators [1,2] presents what is known as the maximum entropy theory of ecology (METE). It consists of finding, through MaxEnt, a joint conditional distribution for the abundance of a species and the metabolic rate of its individuals. From the marginalization and expected values of the MaxEnt distribution, it is possible to obtain (i) the species abundance distribution (Fisher's log series), (ii) the species-area distribution, (iii) the distribution for metabolic rates over individuals, and (iv) the relationship between the metabolic rate of individuals in a species and that species abundance. As novel results, the macrostate entropy is calculated analytically by the Legendre transformation of the log-normalizer in METE. This was previously believed to be unfeasible [1], however as we will see in this talk, the relationship between abundance and metabolic rates and the Lagrange multipliers found when maximizing the entropy can be rewritten as the definition of the Lambert W function [3]. This result allows for a series of analytic results. In this talk I will present the calculation of the metric terms in the information geometry arising from METE and, by consequence, the covariance matrix between METE variables.

References:
[1] J. Harte Maximum entropy and ecology: a theory of abundance, distribution, and energetics. Oxford University Press, 2011.
[2] J. Harte, E.A. Newman. Maximum information entropy: a foundation for ecological theory. Trends in Ecology & Evolution. 29(7), 384-389.
[3] R.M. Corless, D.J. Jeffrey. The LambertW function. In The Princeton Companion to Applied Mathematics, chap. III-17, 151—155. Princeton University Press, 2016

Key Words: Maximum entropy; METE; metabolic rate distributions; information geometry; Legendre transformation; Lambert W function

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An Entropic approach to Classical Density Functional Theory

Ahmad Yousefi and Ariel Caticha
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Density Functional Theory (DFT) was first developed in the context of quantum mechanics and only later extended to the classical regime. The theory was first introduced by Kohn and Hohenberg (1964) as a computational tool to calculate the spatial density of an electron gas in presence of an external potential at zero temperature. Soon afterwards, Mermin provided the extension to finite temperatures. Ebner, Saam, and Stroud (1976) applied the idea to simple classical fluids, and Evans (1978) provided a systematic formulation in his classic paper "The nature of the liquid-vapour interface and other topics in the statistical mechanics of non-uniform, classical fluids.". In this work we derive the classical DFT as an application of the method of maximum entropy. First, the Density Functional formalism is introduced as an extension of the existing ensemble formalisms of statistical mechanics (canonical, grand canonical, etc.) and we show that the core theorem of DFT is an immediate consequence of MaxEnt: we prove that there exists an intermediate density functional entropy S(E, n(x)] which is maximized at the equilibrium density. In a second application of the MaxEnt method, it is then deployed as a systematic approach to generate an optimal approximation from within a family of more tractable trial functionals. (It is already known that mean field theory, and the Bogoliubov method turn out to be special cases of this technique.) As an illustration of the method we recover the main results produced by Evans, and we provide a further extension of the DFT approach through the introduction of information geometry and by working with weighted family of trials.

On inverse problems of Y-DNA genealogy

Arthur Baraov

HP Inc., Russian Federation

There are two major inverse problems in genetic genealogy: (a) estimating time to the most recent common ancestor (TMRCA) for an arbitrary group of males; (b) calibrating Y chromosome microsatellite mutation rates for different marker loci. A comprehensive and uniform Bayesian solution is given for both problems.

Genetic genealogy, Y chromosome, haplogroup, haplotype, STR mutation rates, TMRCA

Bayesian approach to pH measurements in endocytic compartments

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Endocytosis is a mechanism of internalization of extracellular cargo and transmembrane receptors with consequent sorting for recycling and/or degradation. Cargo progression through endocytic compartments is accompanied by decreasing pH from 7.0 to 5.0 [1]. Acidification of endosomes occurs by active proton pumping into endosome lumen. Previous research has shown that inhibitors of endosome acidification (chloroquine, bafilomicine A1) block cargo propagation between endocytic compartments [2,3]. However, precise mechanism of pH regulation in the endosome lumen is unknown. Generally, pH in endosomes is measured via ratiometric approach by internalizing cargos conjugated with pH-dependent and pH-independent fluorophores and measuring the ratio of cargos florescence intensities in endosomes from confocal microscopy images of living cells. Then pH is obtained from the ratio using a calibration curve. The calibration curve is calculated by measuring intensity ratios in fixed cells placed in a buffer with defined pH. Such ratiometric approach combined with artificially pulsed "wave of cargo" revealed many details of pH progression in endocytosis. Unfortunately, this approach provides very wide distribution of intensity ratios which precludes accurate assessment of endosomal pH in more physiological experiments, where cargoes are simultaneously present in endosomal compartments with different pH. In this work, we present method based on a Bayesian approach with entropic prior to derive pH distribution in endosomes. The experimental data were acquired by internalization of mixture LDL-pHRodo and LDL-Alexa488. Surprisingly, our analysis reveals that pH distribution over endosome population consists of well separated narrow peaks. pH of these peaks are well in line with values found in "cargo wave" experiments. The discrete nature of the pH distribution with almost complete absence of intermediate pH values is demonstrated for the first time and suggests the existence of yet unknown regulatory mechanism.

References:
[1] B.Tycko and F. R. Maxfield, Cell, 28(3), 643-651 (1982).
[2] T.Yoshimori et al, JBC, 266(26), 17707-17712 (1991).
[3] M.Mauthe et al, Autophagy, 14(8), 1435-1455 (2018)

Key Words: Parameter inference, Monte Carlo, surrogate model, Gaussian process regression, dimensionality reduction

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Conditional probability, quantum time and friends

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Starting from a minimalistic approach of nature description with only quantum systems and unitary interactions we define conditional probabilities of quantum measurements [1] in the context of the quantum time (also called timeless) formalism. Since its first formulation in 1983 [2], several works investigated on the probability function properties in such a framework. Here we take the advantage of the best both worlds of timeless description of dynamics and Positive-Valued Operator Measurement to provide a coherent description of subsequent measurements. We consider the Wigner's friend measurement scenario where two observers attribute different attributes to a same observed systems. We show that, in the formalism described here, the associated probability expressions can be simply and unambiguously formulated. No paradoxical situations emerge and the roles of Wigner and the friend are completely interchangeable. In particular, Wigner can be seen as a superimposed of states from his/her friend. We demonstrate in addition that, when only one clock system is considered, two-times probabilities cannot be defined (see e.g. Ref. [3,4]) and the causal order is in fact encoded in the considered Hamiltonian, differently than a previous work [5].

References:
[1] M. Trassinelli, Trassinelli, arXiv preprint quant-ph/2103.08903 (2021)
[2] D.N. Page and W.K. Wootters, Phys. Rev. D 27, 2885-2892 (1983).
[3] C.E. Dolby, arXiv preprint gr-qc/0406034 (2004)
[4] V. Baumann et al., arXiv preprint quant-ph/1911.09696 (2019)
[5] M. Trassinelli, Phys. Rev. A 102, 052224 (2020)

Key Words: quantum measurement, quantum time, conditional probabiltiy, Wigner's friend

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David Blower's Legacy

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[2]University of Newcastle, Australia.

David Blower was a very enthusiastic Maxentian. He wrote a series of books with the general title Information Processing and contributed papers to several Max-Entworkshops [1], [2], [3]. He passed away in February 2018. David first got his inspiration from reading all the writings of E. T. Jaynes extremely closely. And in some places he combines great admiration with a sometimes rigorous critiquing of the physicist who originally inspired these MaxEnt meetings.Volumes I, II, and III -with the general title Information Processing-have the respective subtitles Boolean Algebra, Classical Logic, Cellular Automata, and Probability Manipulations (528 pages), The Maximum Entropy Principle (608 pages), and Introduction to Information Geometry (666 pages). There is also available a Supplemental Exercises for VolumeI (401 pages). David was working on his Volume IV at his untimely death. After reading his draft, we feel strongly that the very considerable time and effort he invested in the whole Information Processing series should be complemented by a serious effort to allow his Volume IV (Introduction to Artificial Neural Networks(157 pages)) to "see the light of day". In this Presentation we would like to give you further background on our "Volume IV" project, invoke a discussion about David's earlier books, and enquire of MaxEnt delegates as to whether they had ever had any discussions with David on his project.

References:
[1] Blower, D. (2005). An Easy Derivation of Logistic Regression from the Bayesian and Maximum Entropy Perspective. In Bayesian Inference and Maximum Entropy Methods in Science and Engineering. Erickson, G. & Zhai, Y. (Eds). AIP Conference Proceedings 707, 30-43.
[2] Blower, D. (2007). Cellular Automata Generalized to an Inferential System. In Bayesian Inference and Maximum Entropy Methods in Science and Engineering. Knuth, K.H., Caticha, A., Center, J., Giffin, A. & Rodrigues, C. (Eds). AIP Conference Proceedings 954, 109-116.
[3] Blower, D. (2009). Jaynes's View on the Meaning of "Uninformative" Distributions. In Bayesian Inference and Maximum Entropy Methods in Science and Engineering. Goggans, P. & Chan, C.-Y. (Eds). AIP Conference Proceedings 1193, 20-31.

Key Words: Bayes' Theorem, Maximum Entropy Principle,Neural Network

A weakly informative prior for resonance frequencies

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We derive a weakly informative prior for a set of ordered resonance frequencies from Jaynes' principle of maximum entropy. The prior facilitates model selection problems in which both the values and the number of the resonance frequencies are unknown. It encodes a weakly inductive bias, provides a reasonable density everywhere, is easily parametrizable, and is trivial to sample. We hope that this prior can enable a new class of problems to be attacked with robust evidence-based methods, even in the presence of multiplets of arbitrary order. In our own work, it has enabled very high precision measurements of resonance frequencies of the vocal tract. Other applications include:
-Nuclear magnetic resonance (NMR) spectroscopy [1]
-Resonant ultrasound spectroscopy (a standard method in material science) [2]
-The analysis of atomic spectra [3], such as X-ray diffraction [4]
-Absorption spectral-line finding in astronomy [5]
-Accurate modeling of instrument noise (in this case LIGO/Virgo noise) [6]
-Spectral mixture kernels in Gaussian processes [7]

References:
[1] Andrew Gordon Wilson, Yuting Wu, Daniel J. Holland, Sebastian Nowozin, Mick D. Mantle, Lynn F. Gladden, and Andrew Blake. Bayesian Inference for NMR Spectroscopy with Applications to Chemical Quantification. arXiv:1402.3580 [stat], February 2014.
[2] K. Xu, G. Marrelec, S. Bernard, and Q. Grimal. Lorentzian-Model-Based Bayesian Analysis for Automated Estimation of Attenuated Resonance Spectrum. IEEE Transactions on Signal Processing, 67(1):4-16, January 2019.
[3] Martino Trassinelli. Bayesian data analysis tools for atomic physics. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 408:301-312, October 2017
[4] Chris M. Fancher, Zhen Han, Igor Levin, Katharine Page, Brian J. Reich, Ralph C. Smith, Alyson G. Wilson, and Jacob L. Jones. Use of Bayesian Inference in Crystallographic Structure Refinement via Full Diffraction Profile Analysis. Scientific Reports, 6(1):31625, August 2016.
[5] J. R. Allison, E. M. Sadler, and M. T. Whiting. Application of a Bayesian Method to Absorption Spectral-Line Finding in Simulated ASKAP Data. Publications of the Astronomical Society of Australia, 29(3):221-228, 2012/ed.
[6] Tyson B. Littenberg and Neil J. Cornish. Bayesian inference for spectral estimation of gravitational wave detector noise. Physical Review D, 91(8):084034, April 2015.
[7] Andrew Wilson and Ryan Adams. Gaussian process kernels for pattern discovery and extrapolation. In International Conference on Machine Learning, pages 1067-1075, 2013

Statistical Mechanics of Unconfined Systems: Challenges and Lessons

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In some applications of statistical mechanics, it is undesirable to constrain a system within a finite spatial volume, as one normally does to ensure that the probability distribution on the phase space arising from maximizing the entropy with certain constraints, is normalizable. Examples of such applications include the modelling of a self-gravitating star or the thermodynamics of structure formation in cosmology. We present an exact solution to the maximum entropy problem for assigning a spherically symmetric distribution on the phase space of an unconfined ideal gas in an anti-de Sitter background. Notwithstanding the gas's freedom to move in an infinite volume, the resulting probability distribution is normalizable. We also show that, as in the familiar Minkowski case, there are no stationary, sphericallysymmetric, and normalizable solutions in the static patch of the de Sitter spacetime. In general relativity, the conserved quantities, such as the Arnowitt-Deser-Misner mass, cannot be spatially localized. Worse, they are solely conserved when the backreaction on the metric is accounted for properly. Hence, the conventional use of the total energy as a constraint for extremizing the entropy is untenable on physical grounds. As a part of our analysis, we formulate a novel class of dynamical constraints to circumvent this issue and offer an interpretation in terms of local measurements.

Key Words: Maximum entropy; Unconfined gases; General Relativity; anti-de Sitter spacetime

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Regularization of the gravity field inversion process with high-dimensional vector autoregressive models

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Earth's gravitational field provides invaluable insights into the changing nature of our planet. It reflects mass change caused by geophysical processes like continental hydrology, changes in the cryosphere or mass flux in the ocean. Satellite missions such as the NASA/DLR operated Gravity Recovery and Climate Experiment (GRACE), and its successor GRACE Follow-On (GRACE-FO) continuously monitor these temporal variations of the gravitational attraction. In contrast to other satellite remote sensing datasets, gravity field recovery is based on geophysical inversion which requires a global, homogeneous data coverage. GRACE and GRACE-FO typically reach this global coverage after about 30 days, so short-lived events such as floods, which occur on time frames from hours to weeks, require additional information to be properly resolved. In this contribution we treat Earth's gravitational field as a stationary random process and model its spatio-temporal correlations in the form of a vector autoregressive (VAR) model. The satellite measurements are combined with this prior information in a Kalman smoother framework to regularize the inversion process, which allows us to estimate daily, global gravity field snapshots. To derive the prior, we analyze geophysical model output which reflects the expected signal content and temporal evolution of the estimated gravity field solutions. The main challenges here are the high dimensionality of the process, with a state vector size in the order of 103 to 104, and the limited amount of model output from which to estimate such a high-dimensional VAR model. We introduce geophysically motivated constraints in the VAR model estimation process to ensure a positive-definite covariance function.

From random walks to MaxEnt and back - statistical mechanics and stochastic processes

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Inferring the unknown distribution is the central question of MaxEnt. It is also a question that arises in ecology, spread of epidemics, stochastic processes, and in any problem in general where the unknown is a distribution, whether it is a probability distribution, a distribution of size, of species or any other attribute. The appeal of MaxEnt is that it arrives to the final answer though an improbable shortcut: maximize an appropriate functional under constraints that summarize our knowledge about the process. Unlike problems in statistical inference, many problems in physical science are built around models, sets of rules that specify how the unknown distribution is transformed from a known initial state to a final state some time later. Is it still possible to apply MaxEnt when our knowledge about the process is not a set of constraints but a model? The answer is yes and here we show how. We consider a generic stochastic process that produces a trajectory of transitions in discrete time that represent a random walk in the event space of X starting at known x0. We construct an ensemble of N walkers undergoing such transitions one walker at a time, all walkers starting at the same initial state. At the heart of the theory is a space of distributions that can be produced in a fixed number of transitions and a special functional that assigns probabilities to this space. The maximization of this functional identifies the most probable distribution and generates the mathematical network of thermodynamic relationships. We make contact with Shannon/Gibbs entropy, Kullback-Leibler divergence and elucidate the origin of improper priors in relative entropy. We establish the relationship between stochastic processes and statistical mechanics and demonstrate the theory with examples random walks that exhibit the analogue of phase transitions [1,2].

References:
[1] T. Matsoukas. Generalized Statistical Thermodynamics: Thermodynamics of Probability Distributions and Stochastic Processes. Springer International Publishing, (2019)
[2] T. Matsoukas. Thermodynamics beyond molecules: Statistical thermodynamics of probability distributions. Entropy, 21(9) (2019)

Key Words: Most probable distribution, statistical thermodynamics, stochastic processes

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Getting the Most out of Data: Smart-Data Machine-Learning for Surface Structure Search

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The key challenge for surface structure search is the enormous number of possible polymorphs. Finding the lowest energy polymorph with conventional stochastic algorithms would require an insurmountable computational effort. We overcome this using the quasi-deterministic SAMPLE approach, which is based on smart-data machine-learning and experimental design theory. A few hundred DFT calculations suffice to exhaustively predict the local minima of the potential energy surface. To gain maximal insight from a limited amount of data, we employ an energy model based on molecule-substrate and molecule-molecule interactions. Using Bayesian linear regression, it extracts them directly from formation energies of polymorphs. SAMPLE assigns each interaction a feature based on atom distances. The features differentiate between atom species, allowing to separate contributions of various molecule-fragments to the formation energy, yielding knowledge about why a particular polymorph forms.

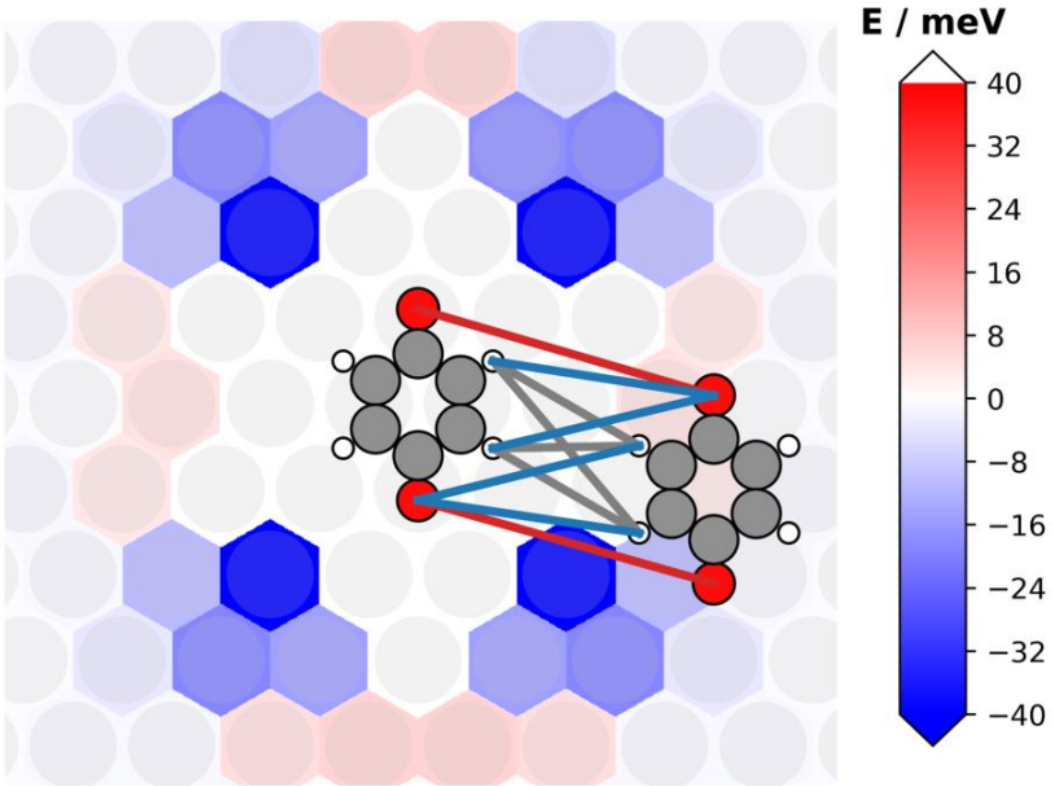

Illustration 1: Interaction energies of two benzoquinone molecules at different respective positions. The lines illustrate the feature assigned to a specific molecule-molecule interaction.

Using Trained Neural Networks for Bayesian Reasoning

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In this talk we present how to combine independently trained neural networks to jointly solve novel tasks through Bayesian reasoning. Deep generative networks serve as prior distributions on complex systems and regression/classification networks are used to check whether certain features are present. Bayes Theorem allows us to then solve the inverse problem in terms of the latent variables of the generator to obtain the distribution of systems that are compatible with one or several posed constraints. We demonstrate how elaborate tasks can be formulated by imposing multiple constraints simultaneously. As Bayesian inference extends logic towards uncertainty, such questions are answered with reason. We show how this approach is compatible with state-of-the-art machine learning architectures with millions of trained weights and hundreds of latent parameters. While traditional machine learning approaches might be better at one specific task, we do not have to train a dedicated network for everything. We flexibly compose appropriate networks from a library of building blocks and solve the associated Bayesian inference problem. Each of these building blocks is simple, serves a single pourpose, and can be reused. The scope of questions we can approach in this fashion grows exponentially with the number of available building blocks. This potentially provides a path to reasoning systems that can flexibly answer complex questions as they emerge.

References:
[1] J. Knollmüller, T. Enßlin, arxiv.org/abs/2001.11031

Key Words: Bayesian Inference, Deep Learning, Generative Models, Reasoning, Conditional Generators

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Orbit classification and global sensitivity analysis in dynamical systems using surrogate models

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Dynamics of many classical physics systems are described in terms of Hamiltonian equations. Commonly, initial conditions are only imperfectly known. The associated volume in phase space is preserved over time due to symplecticity of the Hamiltonian flow. Here we study the propagation of uncertain initial conditions through dynamical systems using (symplectic) surrogate models of Hamiltonian flow maps [1]. This allows fast global sensitivity analysis (GSA) with respect to the distribution of initial conditions and an estimation of local Lyapunov exponents (LLE) [2] that give insight into local predictability of a dynamical system. In Hamiltonian systems LLEs permit a distinction between regular and chaotic orbits. Combined with Bayesian methods we provide a statistical analysis of local stability and sensitivity in phase space for Hamiltonian systems. The intended application is early classification of regular and chaotic orbits of fusion alpha particles in stellarator reactors [3]. The degree of stochastization during a given time period is used as an estimate for the probability that orbits of a specific region in phase space are lost at the plasma boundary. Thus, the approach offers a promising way to accelerate computation of fusion alpha particle losses.

References:
[1] K. Rath et al. Submitted to Chaos (2021)
[2] B. Eckhard and D. Yao. Physica D 65 (1993) 100-108.
[3] C. G. Albert et al. J. Plasma Phys. vol. 86, 815860201 (2020)

Key Words: Gaussian process regression, surrogate model, Lyapunov exponent, sensitivity analysis, Hamiltonian systems

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Bayesian Surrogate Analysis and Uncertainty Propagation

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Uncertainty quantification of simulations has gained increasing attention in the field of Computational Engineering in order to address doubtful parameter choices and assess the models' credibility. Owing to the computational cost of modern day applications and higher dimensional parameter spaces, surrogate models have become a popular tool to propagate input parameter uncertainties to observables resulting from expensive computer simulations. While this practise allows to obtain estimates on simulation uncertainties in the first place, the contribution of the uncertainty of the surrogate itself to the total simulation uncertainty is commonly neglected. This is typically justified by deeming the surrogate to be trustworthy based on heuristic diagnostics, e.g. leave-one-out errors, and largely guided by rules of thumb, e.g. on the convergence of Polynomial Chaos Expansions with the number of samples. However, often this 'convergence' is not achievable within the given computational budget, and there is no rule to quantify 'trustworthiness'. Approaching from a data analysis perspective, Bayesian probability theory lends itself to investigate the uncertainties of the surrogate itself. We assume a given but arbitrary input probability distribution, a given "training" set of computer simulations and a given generalized linear surrogate model that implicitly includes Polynomial Chaos Expansions as a special case. While we assume a Gaussian surrogate-uncertainty, we do not assume a scale for the surrogate uncertainty to be known, i.e. a Student-t. Additionally, we show a simple way to implicitly include spatio-temporal correlations. We end up with semi-analytic formulas for surrogate uncertainties and uncertainty propagation. Lastly, we demonstrate an application to quantify the uncertainties of simulated aortic hemodynamics based on rheological experiments with human blood.

Surrogate-enhanced parameter inference for function-valued models

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We present an approach to enhance performance and flexibility of Bayesian inference of model parameters based on observation of measured data. Going beyond usual surrogate-enhanced Monte-Carlo or optimization methods that focus on a scalar loss, we put emphasis on function-valued input and output of formally infinite dimension. For this purpose, the surrogate models are built on a combination of linear dimensionality reduction and Gaussian process regression for the map between reduced feature spaces. Since the decoded surrogate provides the full model output rather than only the loss, it is re-usable for multiple calibration measurements as well as different loss metrics and consequently allows for flexible marginalization over such quantities. We evaluate the method's performance based on a case study of a riverine diatom model [1]. As input data, this model uses six tunable scalar parameters as well as continuous time-series forcing data of weather and river discharge over a specific year. The output consists of continuous time-series data that are calibrated against corresponding measurements from the Geesthacht Weir station at the Elbe river. Results are compared to an existing model calibration using direct simulation runs without a surrogate [2].

References:
[1] M. Scharfe et al. Ecol. Model. 220, 2173-2186 (2009)
[2] U. Callies et al. Submitted to Environ. Model. Asses. (2021).

Key Words: Parameter inference, Monte Carlo, surrogate model, Gaussian process regression, dimensionality reduction

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Poster Abstracts

On two measure-theoretic aspects of the Full Bayesian Significance Test for precise Bayesian hypothesis testing

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The Full Bayesian Significance Test (FBST) has been proposed as a convenient method to replace frequentist p-values for testing a precise hypothesis. Although the FBST enjoys various appealing properties, the purpose of this paper is to investigate two aspects of the FBST which are sometimes observed as measure-theoretic inconsistencies of the procedure and have not been discussed rigorously in the literature. First, the FBST uses the posterior density as a reference for judging the Bayesian statistical evidence against a precise hypothesis. However, under absolutely continuous prior distributions, the posterior density is defined only up to Lebesgue null sets which renders the reference criterion arbitrary. Second, the FBST statistical evidence seems to have no valid prior probability. It is shown that the former aspect can be circumvented by fixing a version of the posterior density before using the FBST, and the latter aspect is based on its measure-theoretic premises. An illustrative example demonstrate the two aspects and their solution. Together, the results in this paper show that both of the two aspects which are sometimes observed as measure-theoretic inconsistencies of the FBST are not tenable. The FBST thus provides a measure-theoretically coherent Bayesian alternative for testing a precise hypothesis.

References:
[1] Kelter, R. (2020). Analysis of Bayesian posterior significance and effect size indices for the two-sample t-test to support reproducible medical research. BMC Medical Research Methodology, 20(88).
[2] Pereira, C. A. d. B., Stern, J. M. (2020). The e-value: a fully Bayesian significance measure for precise statistical hypotheses and its research program. So Paulo Journal of Mathematical Sciences, 119.

Key Words: Full Bayesian Significance Test (FBST); statistical hypothesis testing; Bayesian inference; e-value; measure-theory

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Entropy-based temporal downscaling of precipitation as tool for sediment delivery ratio assessment

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Many regions around the globe are subjected to precipitation-data scarcity that often hinders the capacity of hydrological modelling. The entropy theory and the principle of maximum entropy can help hydrologists to extract useful information from the scarce data available. In this work we propose a new method to assess sub-daily precipitation features such as duration and intensity based on daily precipitation using the Principle of Maximum Entropy. Particularly in arid and semiarid regions, such sub-daily features are of central for modelling sediment transport and deposition. The obtained features were used as input to the SYPoME model (Sediment Yield using the Principle of Maximum Entropy [1]). The combined method was implemented in seven catchments in Northeast Brazil with drainage areas ranging from 10^{-3} to 10^{+2} km^2 in assessing sediment yield and delivery ratio. The results showed significant improving when comparing with conventional deterministic modelling, with Nash-Sutcliffe Efficiency (NSE) of 0.96 and absolute error of 21% for our method against NSE of -4.49 and absolute error of 105% for the deterministic approach.

References:
[1] Araujo, Jose Carlos de. Entropy-based equation to assess hillslope sediment production. Earth Surface Processes and Landforms, pg 2005-2018 (2007).

Key Words: SDR; Sediment Yield; Downscaling

Global variance as an utility function in Bayesian optimization

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Bayesian optimization explores multi-dimensional variable spaces with target values obtained from expensive black box functions. We employ a Gaussian-process surrogate model based on already acquired data to approximate the unknown target surface and use a mixture of utility functions to optimally locate the next function evaluations in parameter space. While in a previous work [1] we investigated the performance of several utilities like the expected improvement of an additional data point or the data point with the maximal variance, this paper proposes to consider the global variance, i.e. to integrate the function uncertainty over a finite parameter space volume. It turns out that this utility function not only provides a tool set for fine tuning the investigations in the region of interest but expedites the optimization procedure in toto.

References:
[1] R. Preuss and U. von Toussaint, "Optimization employing Gaussian Processbased Surrogates", in "Bayesian Inference and Maximum Entropy Methods in Science and Engineering", Proceedings of the 37. International Workshop, ed. A. Polpo, J. Stern, F. Louzade, R. Izbicki, H.H. Takada, Springer Proc. in Math. Stat.239, 275–284, (2018).

Key Words: global optimization, Bayesian optimization, utility, global variance

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Bayesspray - analysis of electrospray mass spectrometry data using nested sampling

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The Electrospray Revolution [1] in mass spectrometry (MS) began in the late 1980s with the publication of spectra showing multiply-protonated proteins. Large molecules often have masses lying outside the range directly accessible by some mass spectrometers. Because these instruments measure mass-to-charge ratios however, the effective mass range increases with the number of charges on a molecule. A potential downside of electrospray ionisation is the distribution of charge states obtained, which often significantly increases the complexity of the data (especially for complex mixtures). By the early 1990s, Maximum Entropy based deconvolution [2] had in turn revolutionised the analysis of electrospray MS data, and it has remained the gold standard ever since. It now enjoys countless applications in biology, biotheraputic drug development and quality control, and polymer analysis among many others. Recent algorithmic advances [3] and the advent of higher-resolution mass spectrometers motivated the development of a next-generation Bayesian algorithm BayesSpray which has a performance exceeding that of MaxEnt based methods and applicability to a wider range of data. We describe this algorithm and give some examples of its use in emerging applications such as oligonucleotide analysis and protein theraputics.

References:
[1] J. Fenn, Electrospray Wings for Molecular Elephants, Nobel Lecture (2002)
[2] A.G. Ferrige, M.J. Seddon, B.N. Green, S.A. Jarvis and J. Skilling, Disentangling Electrospray Spectra with Maximum Entropy, Rapid Commun. Mass Spectrom. 6, 707-711 (1992).
[3] J. Skilling, Nested Sampling for General Bayesian Computation, Bayesian Anal. 1(4), 883-859 (2006)

Key Words: Nested Sampling, mass spectrometry

Clustering methods for exploration of potential energy surfaces

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Although much heavier than electrons, light nuclei, mainly hydrogen, exhibit Nuclear Quantum Effects, such as tunnelling, that can have a large impact on the structure and the dynamics of materials [1]. The standard method to account for them when simulating the static properties at equilibrium is path integrals. However, this method considerably increases the number of degrees of freedom, making the exploration of the potential energy landscape much harder. Our goal is therefore to reduce the number of sampling points. To do so, we use nested sampling, which turns the multi-dimensional problem into a one-dimensional integral, thus considerably reducing the computational needs for sampling. We aim to implement other exploration methods in Nested fit [2] in addition to the random walk, presently implemented for the search of new sampling points (live points). The recognition via machine learning methods of cluster structures of the live points, corresponding to the function minima, will allow to focus on specific regions that mostly contribute to the energy landscape. Here, we aim to compare the different cluster analysis methods implemented and under development in Nested fit and assess their performances on synthetic and real problems. In particular, these techniques will be tested with the benchmark case of the molecular potential of Lennard-Jones atomic clusters.

References:
[1] Y. Bronstein, P. Depondt and F. Finocchi, Thermal and nuclear quantum effects in the hydrogen bond dynamical symmetrization phase transition of δ-AlOOH, Eur. J. Mineral. 29 (2017), 1.
[2] M. Trassinelli and P. Ciccodicola, Mean shift cluster recognition method implementation in the nested sampling algorithm, Entropy 22 (2020), 185.

Key Words: Nuclear Quantum Effects, Nested Sampling, Clustering, Lennard Jones

Bayesian-assisted strategies to Landau-like effective Hamiltonians

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Many crystals undergo order-disorder transitions, which can be conveniently described via Landau-like Hamiltonians [1]. However, the order parameter usually couple with other degrees of freedom and the coupling may be highly non linear. The construction of effective Hamiltonians containing a reduced number of degrees of freedom is therefore non trivial. Nevertheless, those effective Hamiltonians are highly desirable, as they can be solved in the thermodynamic limit and including Nuclear Quantum Effects (NQE), such as zero-point energy and tunneling. These effects are crucial for certain materials with light nuclei, and are computed via path integrals, inflating the dimensionality of the problem, and consequently increasing the computation time for exploring energy landscapes. In order to overcome this bottleneck, here we implement the construction of effective Hamiltonians for the specific case of NaOH and KOH crystals, for which there is a ferroelectric-paraelectric phase transition, using Bayesian model selection methods. First, we choose a finite number of degrees of freedom and compute the potential energy surface (PES) via the Density Functional Theory (DFT). Second, several analytic forms for the PES are proposed and their bayesian evidence are computed through the nested fit [2,3], which implements the Nestled Sampling algorithm. The best model is chosen as the one that maximizes evidence, i.e. the probability of the model itself. Finally, we will employ a similar strategy in order to obtain the smallest set of degrees of freedom that are coupled to the order parameter. The end goal is to find the simplest and most accurate effective Hamiltonians able to reproduce the data, which we will use in computationally-expensive path-integral calculations at finite temperature.

References:
[1] W. Zhong, D. Vanderbilt, and K. M. Rabe, Phys. Rev. Lett. 73, 1861 (1994); Phys. Rev. B 52, 6301 (1995).
[2] M. Trassinelli, Nucl. Instrum. Methods B408, 301 (2017).
[3] M. Trassinelli and P. Ciccodicola, Entropy 22, 185 (2020).

Key Words: Nestled sampling, Nuclear quantum effects, Density functional theory

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