DY 46: Poster: Machine Learning and Data Analytics

Time: Thursday 13:00–16:00 Location: P1

DY 46.1 Thu 13:00 P1

Time series analysis of loudness fluctuations in musical performances and psychophysical experiments — •Benjamin Schulz[1,2], Corentin Nelias[1,2], and Theo Geisel[1,2,3] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Physics Dept., Georg-August University, Göttingen, Germany — [3]Bernstein Center for Computational Neuroscience, Göttingen, Germany

Over the last decades, the study of fluctuations in musical time series showed power spectral densities that exhibit a $1/f^{\beta}$-shape across certain frequency regions, indicating long range correlations. So far time series of pitch, rhythm, or timing were investigated across different musical epochs, composers and styles, showing a variety of β-values between 0 and 2. Whether the fluctuations of musical dynamics, or in other words loudness fluctuations, have similar spectral properties, is an open question, however. We have carried out in-depth studies of manually recorded data sets in different musical settings. A first set results from psychophysical tapping experiments. A second one consists of drum performances recorded in a musical environment. All participating musicians were professionals. The tapping and drumming data consistently show the clear occurrence of a $1/f^{\beta}$-shape in the power spectral density. Furthermore, the presence of a metronome click in the tapping experiment leads to the strengthening of specific periodic structures in the loudness fluctuations and also seems to have an impact on the coefficient β.

DY 46.2 Thu 13:00 P1

Battery modeling: Fusing equivalent circuit models with data-driven surrogate modelling — •Limei Jin[1,2], Franz P. Bereck[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]IEK-9, Forschungszentrum Jülich, Jülich, Germany

Electrochemical impedance spectroscopy (EIS) is widely used to characterize electrochemical energy conversion systems. The traditional analysis with equivalent circuit models (ECM) has recently been augmented by a transform based distribution of relaxation times (DRT) analysis which allows one to reduce the ambiguity in the construction of ECMs and thus overfitting. Experimentally determined ECM parameters vary depending on operating conditions and the lifetime history of battery usage. Here we focus on State of Health (SOH) and State of Charge (SOC) as a basis for operando diagnosis and functionality optimization in the setting of fast-charging. Within pure ECM approaches, aging effects can only be represented to a limited extent, as aging is related to a variety of different factors whose impact on cell impedance are not sufficiently understood, yet. The highly complex interplay of factors motivates the development of data-driven Machine Learning (ML) models as a basis for future battery management systems. We present ML enabled ECMs based on experimental impedance analyses and a data-driven ML approach that computationally samples an abstract target space for classification and recognition of cells at vastly different SOC/SOH combinations.

DY 46.3 Thu 13:00 P1

Machine learning categorization of the Anderson model — •Quangminh Bui-Le and Rudolf Römer — Department of Physics, University of Warwick, Coventry, CV4 7AL

Machine learning (ML) methods have been used to identify phase transitions of physical systems by categorizing systems based on the Ψ^2 values of their wave-functions into extended and localized states, which a model is then trained on in order to identify between the extended and localized states. Here we want to see if ML is powerful enough to categorize systems into even more specific groups by attempting to categorize Anderson model data into categories based on the disorder of the wave-function. We are using a PyTorch model to create a convolutional neural network using a ResNet18 model. This model will be trained on 3D Anderson model Ψ^2 values from 17 disorder values spanning a range of 15 to 18.

DY 46.4 Thu 13:00 P1

Neural-network based Monte Carlo Markov chain simulation of spin glasses — •Michael Engbers and Alexander K. Hartmann — Carl von Ossietzky University, Oldenburg, Germany

Spin glasses exhibit a complex equilibrium and non-equilibrium behavior at low temperatures. The reason is the existence of an energy landscape with many local minima and high barrieres. In computer simulations, this leads to long correlation times when investigating large systems. Due to this numerical hardness, the model has motivated the development of many new algorithmic approaches like generalized Wolff cluster algorithms, parallel tempering or genetic algorithms.

Recently, it has been shown that the application of generative neural networks can accelerate Monte Carlo simulations, also for simple spin models with apparently promising results.

Here, we use an autoregressive distribution estimator (NADE) to perform a Monte Carlo simulation of spin glasses [1]. We embedded the NADE into a Metropolis-Hastings Markov-chain approach, therefore ensuring detailed balance. We confirm previous results that the acceptance rates of the NADE approach surprisingly increase with decreasing temperature. Nevertheless, we show that crucial observables, such as the distribution of spin overlaps, indicate that this neural-network approach suffers from the lack of effective ergodicity.

[1] B. McNaughton, M.V. Milosević, A. Perali, and S. Pilati, Phys. Rev. E **101**, 053312 (2020).

DY 46.5 Thu 13:00 P1

Influence of mode-coupling on the information processing rate of Spin-VCSEL reservoir computer — •Lukas Mühlnickel, Lina Jaurigue, and Kathy Lüdge — Institut f. Physik, Technische Universität Ilmenau, Weimarer Str. 25, 98684 Ilmenau, Germany

The relative simplicity of reservoir computing, when comparing it to other machine learning methods, makes it suitable for efficient hardware implementation. The needed high dimensional reservoir dynamics can be provided by adding feedback to only one single nonlinear node, while driving the system with time multiplexed inputs. One promising realization utilizes the fast polarization dynamics of power efficient Spin-VCSELs. These fast field interactions are related to birefringence, dichroism and electron transition rates in the cavity material and occur on shorter time scales than the relaxation oscillations. Thus, compared to typical semiconductor lasers, much higher cutoff frequencies in the system response are observed for the Spin-VCSELs. We investigate the influence of these fast polarization oscillation dynamics on the reservoir performance when increasing data processing rates.

DY 46.6 Thu 13:00 P1

Deep learning-based clogging prediction in outflow of hard and soft grains — •Seddigheh Nikipar, Dmitry Puzyrev, Jing Wang, and Ralf Stannarius — Institute of Physics and MARS, Otto von Guericke University Magdeburg, Universitätsplatz 2, D- 39106 Magdeburg, Germany

Studying the outflow of granular materials has been recognized as a challenging topic in physics due to their unexpected behavior, such as segregation, blockage, and other dynamical events [1]. In particular, the early detection of clogging during discharge of granular materials through narrow orifice in silo has significant challenges. In this work, the possibility of early prediction of clogging was investigated through implementation of image-based deep learning approach, which turns out to be a promising strategy to predict the time until the next clog [2]. For this purpose, experiments on discharge of mixtures of hard and soft spheres from a quasi-two dimensional (2D) silo have been conducted [3]. The image dataset of flowing particles was used to train the Convolutional Neural Networks of various architectures and to CNN-LSMT architecture specifically designed for time series analysis. The trained networks demonstrate considerable accuracy in clogging prediction.

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[1] Perge C, et al. Phys. Rev. E 85 021303 (2012) [2] Hanlan J, APS March Meeting, abstract id.M09.010 (2022) [3] J Wang, et al. Soft Matter, 17, 4282 (2021)

DY 46.7 Thu 13:00 P1

Optical reservoir computing with incoherent optical memory — •Mingwei Yang[1,2], Elizabeth Robertson[1,2], Leon Messner[1,3], Norman Vincenz Ewald[1], Luisa Esguerra[1,2], and Janik Wolters[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute of Optical Sensor Systems, Berlin, Germany. — [2]Technische Universität Berlin, Berlin, Germany. — [3]Humboldt-Universität zu Berlin, Berlin, Germany.

Reservoir computing is a machine learning method that is particularly suited for dynamic data processing. A fixed reservoir projects the input information to a high-dimensional feature space, and only the readout weights need to be trained, allowing fast data processing with low energy consumption [1,2]. In this work, we demonstrate an optical reservoir computing using incoherent memory in a cesium vapor cell to predict time-series data. The information is stored in the reservoir by controlling the pump and probe process on the Cs D2 transitions. The coupling between the reservoir and both the input and output data is realized by acousto-optic modulators. [1] G. Tanaka, T. Yamane, J. B. Héroux, R. Nakane, N. Kanazawa, S. Takeda, H. Numata, D. Nakano, and A. Hirose, *Recent advances in physical reservoir computing: A review,* Neural Networks 115, 100*123 (2019). [2] L. Jaurigue, E. Robertson, J. Wolters, and K. Lüdge, *Photonic reservoir computing with non-linear memory cells: interplay between topology, delay and delayed input,* in Emerging Topics in Artificial Intelligence (ETAI) 2022, vol. 12204 (SPIE, 2022), pp. 61*67.

DY 46.8 Thu 13:00 P1

Metadynamics Simulations of Chemical Reactions in Solution — •Azad Kirsan, Sagarmoy Mandal, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer Chemistry Center, FAU Erlangen-Nürnberg, Germany

For four important chemical reactions we have benchmarked two different method for reconstructing the free energy surface (FES) and for estimating the free energy barrier from *ab initio* molecular dynamics (AIMD) simulations: standard metadynamics (MTD) and the recently introduced well-sliced metadynamics (WS-MTD) approach [1], which is a combination of umbrella sampling and MTD. The chosen reactions are a Diels-Alder reaction, an aromatic decarboxylation, an aromatic Claisen rearrangement, and the base-catalyzed hydrolysis of formamide. This selection includes a cycloaddition, an elimination, an intermolecular rearrangement, and an OH^- addition, thus covering a wide range of different reaction types and mechanisms. By utilizing our recently improved version of the CPMD code [2] it was possible to obtain many ns long trajectories of the reactions in the gas phase as well as in an explicitly included solvent.

[1] S. Awasthi, V. Kapil, N. Nair, J. Comput. Chem. **37** (2016) 1413
[2] T. Klöffel, G. Mathias, B. Meyer, Comput. Phys. Commun. **260** (2021) 107745

DY 46.9 Thu 13:00 P1

Analyzing Extreme Fluctuations of the Randomly Forced Nonlinear Schrödinger Equation via Large Deviation Theory — •Sumeja Bureković[1], Tobias Schäfer[2], and Rainer Grauer[1] — [1]Institute for Theoretical Physics I, Ruhr-University Bochum, Germany — [2]Department of Mathematics, College of Staten Island, Staten Island, United States of America

Recently, the focusing nonlinear Schrödinger equation with additive noise has been proposed as a model for finite-time singularity mediated turbulence [1]. Among other findings, the authors of [1] show through direct numerical simulations that the statistics of quantities such as the energy dissipation rate and structure functions are intermittent. Here, in order to explain these observations and to quantify the effect of extreme fluctuations on the turbulence statistics, we employ methods from large deviation theory or instanton calculus [2]. In the first step, the probability density function or expectation for the quantities of interest is approximated by the Freidlin-Wentzell action of the large deviation minimizer or instanton. Additionally, our aim is to improve this approximation by taking into account Gaussian fluctuations around the instanton, harnessing the techniques of [3].

[1] Josserand, C., Pomeau, Y., & Rica, S. (2020). Phys. Rev. Fluid, 5(5), 054607. [2] Grafke, T., Grauer, R., & Schäfer, T. (2015). J. Phys. A Math. Theor., 48(33), 333001. [3] Schorlepp, T., Grafke, T., & Grauer, R. (2021). J. Phys. A Math. Theor., 54(23), 235003.

DY 46.10 Thu 13:00 P1

Light propagation in media with electric and magnetic disorder: 3D Anderson localization — •Walter Schirmacher[1,2], Thomas Franosch[3], Marco Leonetti[1,4], and Giancarlo Ruocco[1,5] — [1]Istituto Italiano di Tecnologia, Roma, Italy — [2]Universität Mainz, Mainz, Germany — [3]Universität Innsbruck, Innsbruck, Austria — [4]SLML, Consiglio Nationale delle Richerche, Roma, Italy — [5]Universita "La Sapienza", Roma Italy

We consider Maxwell's equations in a 3-dimensional material, in which both, the electric permittivity, as well as the magnetic permeability, fluctuate in space. Differently from all previous treatments, we transform the fields in such a way that the linear operator in the equations is manifestly Hermitian, in order to deal with a proper eigenvalue problem. We use an appropriate version of the Coherent-Potential approximation (CPA) to calculate the density of states and scattering-mean-free path. We find that in the presence of both electric and magnetic disorder the spectral range of Anderson localization appears to be much larger than in the case of electric (or magnetic) disorder only.