# DY 34: Poster: Machine Learning, Data Science, and Reservoir Computing

Time: Wednesday 15:00–18:00 Location: Poster C

DY 34.1 Wed 15:00 Poster C

**A First Approach to Dynamically Solving Quadratic Unconstrained Optimization Problems with Memristive Oscillator Networks** — •Bakr Al Beattie and Karlheinz Ochs — Chair of Digital Communication Systems, Ruhr University Bochum, 44801 Bochum, Germany

In recent years, a new computational paradigm based on a network of resistively coupled oscillators has emerged. These devices are referred to as oscillator-based optimizers. They are built, so they have the natural tendency of minimizing an energy function to which quadratic unconstrained binary optimization problems (QUBOs) can be mapped. A challenge of oscillator-based optimization is that the structure of the oscillator network must be changed every time a new QUBO is mapped. This is because the connectivity of the network encodes the coefficients of the optimization problem. To deal with this issue, we propose making use of memristors (memory resistors), which can switch between multiple resistance states. To utilize these devices, it is usually required to have a dedicated programming circuit to set the desired resistance state. In this work, we aim to show that we can omit on using such programming circuits by working with suitable oscillators. To demonstrate this approach, we iteratively solve multiple optimization problems, where we alternate between a programming phase and a solution phase.

DY 34.2 Wed 15:00 Poster C

**Optical Ising model simulations with caesium vapor cells** — •Kilian Junicke[1], Elizabeth Robertson[1,2], Mingwei Yang[1,2], Inna Kwiatkowski[2,3], and Janik Wolters[1,2] — [1]Technische Universiät Berlin, Institute for Optics and Atomic Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR), Rutherfordstr. 2, 12489 Berlin, Germany — [3]TU Berlin, Institut für Luft und Raumfahrt

Several computationally hard optimization problems can be mapped to finding the ground state of an Ising model [1]. Simulating Ising models optically promises speed increases [2]. Building an optical Ising machine then raises the question of how to simulate the spin states [3].

Here we present a scheme for simulating an Ising model using the ground states of cesium vapor at room temperature. We present methods for implementing positive and negative interactions using a measurement and feedback strategy. In the system electromagnetically induced transparency acts as a frequency transducer. We initialize the system and allow it to evolve by executing a series of pump probe operations on spatially multiplexed regions of an atomic vapor cell until a ground state solution is found.

[1] Lucas, A. Ising formulations of NP problems. Front. Phys. 2, 5 (2014).

[2] McMahon, P.L. Physics of optical computing. Nat Rev Phys 5, 717-734 (2023).

[3] Böhm et al. Poor man's coherent Ising machine for optimization. Nat Commun 10, 3538 (2019).

DY 34.3 Wed 15:00 Poster C

**Exploring neural criticality through the structure of input-induced attractors in random neural networks under external perturbations** — •Hiromichi Suetani[1,2] and Ulrich Parlitz[3,4] — [1]Faculty of Science and Technology, Oita Univerisyty, Oita, Japan — [2]International Research Center for Neurointelligence, The University of Tokyo, Tokyo, Japan — [3]Max Planck Research Group Biomedical Physics, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [4]Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany.

In recent years, a focus has turned to the neural criticality hypothesis, suggesting that the neural system optimizes information processing by maintaining activity near a critical point between order and disorder. Reservoir computing (RC) provides a theory for the neural criticality. For example, the hyperparameter region with the maximum Lyapunov exponent (LE) near zero, termed the "edge of chaos," claims the optimality of the performance of RC. Yet, reservoirs are non-autonomous dynamical systems with external perturbations. The maximal LE is defined for autonomous systems and if applied to non-autonomous systems, it is the conditional LE where its positivity and negativity doesn't generally indicate the existence of chaos.

This study explores input-induced attractors in random neural networks under external inputs. Examining them through generalized synchronization and embeddings, we aim at developing a new theoretical foundation for neural criticality by elucidating the relationship with performances of RC such as information processing capacity.

DY 34.4 Wed 15:00 Poster C

**Physical interpretation of learning dynamics in neural networks** — •Yannick Mühlhäuser[1,2], Max Weinmann[2,3], and Miriam Klopotek[2] — [1]University of Tübingen, Tübingen, Germany — [2]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [3]University of Stuttgart, Interchange Forum for Reflecting on Intelligent Systems, IRIS3D, Stuttgart, Germany

Neural network-based machine learning methods are becoming ubiquitous for applications to physics and science. A key challenge for their seamless integration into science is their opacity, or "black-box-ness". How they learn, i.e. their learning dynamics, can shed some light into their "reasoning" process. We look at the learning dynamics of autencoder-type neural networks trained via different optimization techniques [1]. We use statistical model systems for finding specific analogies to well-known phenomena from physics like phase transitions [2], offering a route towards interpretation.

[1] Borysenko, O., and Byshkin, M. (2021). CoolMomentum: A method for stochastic optimization by Langevin dynamics with simulated annealing. Scientific Reports, 11(1), 10705.
[2] Liu, Z., Kitouni, O., Nolte, N. S., Michaud, E., Tegmark, M., and Williams, M. (2022). Towards understanding grokking: An effective theory of representation learning. Advances in Neural Information Processing Systems, 35, 34651-34663.

DY 34.5 Wed 15:00 Poster C

**Understanding Neural Network Models for Phase Recognition** — •Shashank Kallappara, Janett Prehl, and Martin Weigel — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

The Ising model is one of the best-known models in statistical physics, undergoing a phase transition in dimensions $d > 2$, described by a simple order parameter: its magnetisation. Machine learning techniques have been successfully used in physics for classifying phases of different physical systems. Fully connected neural networks have been shown to learn the translational invariance of the Ising model when learning its phases using only a single hidden layer; analytic solutions for the same exist for highly compact networks that are constructed to obey the translational invariance automatically. Here, we show this learning of the invariance in single-layer networks of different widths and compare the networks' performance in classifying the phases. We also consider a highly compact network but focus on the gradient descent learning dynamics over its loss landscape; we suggest a few changes to this that greatly improve its performance while preserving interpretability.

DY 34.6 Wed 15:00 Poster C

**Sand Grain Generation through Deep Learning and Lower Dimensional Representations** — •Lira Yelemessova[1] and Matthias Schröter[1,2] — [1]Georg-August-Universität Göttingen, Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

How would one create artificial realistic sand grains? This project explores this question by representing sand grains as point clouds and then employing the denoising diffusion probabilistic model. The first step is to use an autoencoder to transform the complex three-dimensional structures of synthetic sand grains into a lower-dimensional space. Then, the model generates additional samples using denoising diffusion, which is also the algorithm behind programs such as Stable Diffusion and DALL-E. We study how variations in the number of points and dimensions of additional features impact the generated samples.

DY 34.7 Wed 15:00 Poster C

**Squeezing Sand Grains through a Bottleneck: Can Deep Learning Find a Minimal Description for Granular Particles?**

— •Azhar Akhmetova[1] and Matthias Schröter[1,2] — [1]Georg-August-Universität Göttingen, Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

The optimal number of parameters required for reliably describing a specific class of shapes is an open question. We test the possibility of retrieving the minimum number of parameters needed using the autoencoder architecture. Autoencoders are neural networks consisting of two parts: the encoder that compresses input data into a lower-dimensional representation, creating an information bottleneck. Then, the decoder reconstructs the original input from this compact representation. We start by applying autoencoders to shapes generated with a known parameter count based on their Fourier descriptors. The focus is on testing if the autoencoder's bottleneck dimension can measure the required number of parameters. Another open question is how the resolution influences particle shape description. The final aim of the project is to apply autoencoders on X-ray tomography data of real-world particles.

DY 34.8 Wed 15:00 Poster C

**Mutual information estimation in the learning process of neural networks** — •Lea Melina Faber, Ibrahim Talha Ersoy, and Karoline Wiesner — Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland

Deep neural networks play an increasingly important role to predict the dynamics of highly complex systems. The most prominent example is that of climate models. Nonetheless it is still unknown how the actual learning process works. To better understand such models it is crucial to open the black box of neural nets. It has been conjectured, that mutual information is a good measure of learning in neural networks. Often times the simplest of estimation techniques, like binning, are used. However, it has been shown that in some settings they are only very crude estimators. We have analyzed the MSE, bias and variance for standard mutual information estimators, using the specific settings relevant for neural network analysis. Our results show that most estimators have problems with high dimensions and high mutual information, specifically in combination, which is a standard situation in the context of neural networks. Furthermore, it has been shown, that generally estimators show the best results for Gaussian distributions. However, our numerical experiments show that non-Gaussian distributions are likely to play a significant role in the learning processes in neural networks. Hence, we require suitable estimators for these cases. We illustrate our results with the MNIST dataset.

DY 34.9 Wed 15:00 Poster C

**Cumulative entropy as a bridge between statistical physics and statistical machine learning** — •Hans Reimann and Karoline Wiesner — University of Potsdam, Germany

Cumulative entropies, such as cumulative Shannon entropies or Phi-entropies, have been of growing interest to tackle shortcomings of classical notions of entropy while keeping as many of the desired properties as possible. Some context driven intuitions and overarching frameworks managed to provide some independent insights, yet they are not fully understood or incorporated in well established physical or statistical contexts is still work in progress. We investigate towards statistical and physical properties as well as understanding of the cumulative paired Shannon entropy (CPE) as a promising special case. Utilizing tools from mathematical statistics in combination with information theory our work paves the way toward a thorough understanding along the lines of well established notions of entropy. Next to some first results on parametric and non-parametric estamation and asymptotic properties, we managed to relate the CPE in its most striking properties to both concpets of equilibrium statistics and thermodynamics as well as statistical data analysis. Moreover, we work on expanding these ideas to recent results in physics informed machine learning for binary classification tasks via arguing for the CPE to be a measure of a natural degree of seperability under considerations of Jaynes' understanding of maximum Shannon entropy.

DY 34.10 Wed 15:00 Poster C

**Phase Transitions and Information Flow in Deep Neural Networks** — •Ibrahim Talha Ersoy[1] and Karoline Wiesner[2] — [1]Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland — [2]Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland

The learning process of neural networks (NNs) can be characterized as an optimization toward specific balance between complexity of the representa- tion and precision, both of which can be measured by the mutual informa- tion. This observation as well as the so called information bottleneck (IB) approach where one restricts complexity goes back Tishby et al. [1,2]. In the IB approach two mutual information terms are built into the loss function, with some trade-off parameter giving their balance. It was observed that the system undergoes a number of second order phase transitions when varying this parameter [3]. We utilize this feature to better understand the change between different model representations. A close connection to schemes like the variational autoencoder and other networks with variable regularizes has been suggested [5]. We investigated these claims and make a number of trials and theoretical considerations to make this claim manifest. In particular we probed the dependencies of hidden representations and the features they represent. We also compared the compression behaviour of the NN-input to other methods like PCA, Diffusion maps and t-SNE. For gaussian data we see a strong connection between the VAE, IB as well as PCA, as expected.

DY 34.11 Wed 15:00 Poster C

**Ab-initio-based interatomic potential for laser-excited Bismuth** — •Jimiben Patel, Bernd Bauerhenne, and Martin Garcia — Institute for Physics, University of Kassel, Kassel, Germany

The intricate processes involving atomic motions, occurring on a subpicosecond timescale, influence phenomena like chemical reactions, bond formation, and breaking. To get deep insights into these processes, femtosecond laser pulses have proven indispensable. The ultrashort interaction time in this context ensures that the laser field strongly influences electrons. A precise description of the structural relaxation of materials after femtosecond laser excitation is achieved through Te dependent Density Functional Theory (DFT). However, employing Te dependent DFT for simulations involving a large number of atoms is computationally expensive or even impossible. To address this challenge, our work introduces a polynomial Te dependent interatomic potential ($\Phi$(Bi)(Te)) for Bismuth, which is trained using a database constructed from DFT simulations. Bismuth is an experimentally widely used material, for which so far no theory to describe ultrafast processes has been developed. In our analysis, we compared the physical properties of our polynomial potential $\Phi$(Bi)(Te), with those obtained from ab initio simulations. Additionally, we conducted an examination of the thermophysical properties of the polynomial potential, including the determination of the melting temperature. This innovative approach allows for efficient and accurate exploration of complex material behaviors, offering a valuable alternative to computationally demanding Te dependent DFT simulations.

DY 34.12 Wed 15:00 Poster C

**Long-Range Electrostatic Descriptors for Machine Learning Force Fields** — •Carolin Faller[1,2], Bernhard Schmiedmayer[1], and Georg Kresse[1,3] — [1]Computational Materials Physics, University of Vienna, Austria — [2]Vienna Doctoral School in Physics, University of Vienna, Austria — [3]VASP Software GmbH, Vienna, Austria

We present flexible and physically meaningful descriptors for modeling long-range electrostatic interactions in machine learning force fields (MLFFs).

While local, atom-centered descriptors can accurately describe properties of several materials, they completely disregard long-range effects. For example long-range electrostatics are a crucial aspect of ionic materials, which makes it necessary to develop new techniques that account for them in order to ensure the predictive capability of MLFFs.

Our novel descriptors account for long-range interactions without resorting to a global description. They characterize the atomic density, similar to commonly used short-range methods. Periodic images of all atoms are accounted for by calculating the atomic density in reciprocal space.

This new long-range model is comparable to the long-distance equivariant (LODE) framework [1] for system with purely electrostatic interactions. Our model outperforms LODE in predicting energies and forces for real materials, where local approaches fall short.

[1] A. Grisafi, The Journal of Chemical Physics, **151**, 204105 (2019).

DY 34.13 Wed 15:00 Poster C

**Feedback Controlled Microscopy Using Machine Learning** — •M Asif Hasan and Frank Cichos — Faculty of Physics and Earth System Sciences, Leipzig University, Linnéstraße 5, Leipzig, Germany

Feedback control is crucial in stabilizing unstable states, evident in living organisms to regulate system functions and in technological applications like quantum state control. The combination with ma-

chine learning offers novel approaches to probe and manipulate complex physical or chemical processes, where machine learning algorithms determine the control strategy for inducing specific physical or chemical perturbations in a microscopic system. Our project investigates a more cohesive approach to feedback-controlled microscopy, particularly in steering active microparticles amidst complex, noisy environments. To this end, we integrate a microscope and laser steering system with real-time particle detection and machine learning enabled feedback algorithm, specifically, the Actor-Critic Reinforcement Learning (ACRL) approach. We show that the AI agent can navigate the active particles and complex mixtures of passive particles to a target state with high precision, amidst environmental uncertainties such as Brownian motion and flow fields. With a multi-agent real-time learning design, we focus on navigating, adapting, and optimizing behaviors under fluctuating conditions, enabling the agents to proficiently interpret sensory data and learn optimal response policies in continuous action spaces. This study therefore paves the way to develop a universal Actor-Critic Reinforcement Learning multi-agent system enabling high-precision control in noisy settings of various fluidic scenarios.

DY 34.14 Wed 15:00 Poster C

**Atomistic Simulations of Laser-Excited Carbon with Convolutional Neural Network Interatomic Potentials** — •Luc Wieners, Bernd Bauerhenne, Malwin Xibraku, and Martin E. Garcia — University of Kassel

Atomistic simulations in solid state physics are usually done with density functional theory (DFT). While DFT has a great accuracy, its computation time scales cubical with the size of the system due to the high computational cost of solving the Kohn-Sham equations. Therefore we look at a faster approach which uses machine learning with neural networks to replicate DFT results. We build a machine learning interatomic potential and train it to predict atomic forces based on DFT calculations. This neural network interatomic potential can be used for MD simulations of laser-excited carbon due to the high accuracy of its force predictions. At the same time, the computational cost of this potential scales linear with the system size, enabling simulations of large systems and long time spans which cannot be simulated with DFT. In this work we focus on convolutional neural networks which allow the direct processing of the atomic structure as an image which speeds up the calculation of the network input.

DY 34.15 Wed 15:00 Poster C

**Machine Learning the Anderson model of localization** — Djénabou Bayo[1,2] and •Rudolf A. Römer[1] — [1]Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom — [2]Laboratoire de Physique Théorique et Modélisation (LPTM) (CNRS UMR8089), CY Cergy Paris Université, 95302 Cergy-Pontoise, France

In recent years, we witnessed the emergence of DNN techniques in several fields of physics as a new tool for data analysis. In condensed matter physics in particular, DNN and CNN proved to be performing well in identifying and classifying the phases of matter or learning order parameters. The Anderson model of localization is characterised by a phase transition from a metal state (with an extended wave function) to an insulator (with a localised wave function) in the presence of high disorder. This model was previously studied by T. Ohtsuki et al. and it was shown that ML techniques were able to distinguish the two phases. In our study, we employ a ResNet18 to reconstruct the full disorder resolution from normalised eigenstates $\psi$. We find that given large enough system sizes $L^3 > 40^3$, classification methods are able to make acceptable predictions on the disorder. Furthermore, we show that by using a reduced number of trained disorder values, regression methods are able to make good predictions on a larger set of disorders. Our implementation was made by using the PyTorch library.

DY 34.16 Wed 15:00 Poster C

**Bridging the Gap: From EIS to Real-World Battery Performance with Stochastic Pulse Design** — •Limei Jin[1,2], Franz Bereck[2], Josef Granwehr[2], Rüdiger-A. Eichel[2], Karsten Reuter[1], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]IEK-9, Forschungszentrum Jülich

While Electrochemical Impedance Spectroscopy (EIS) offers valuable insights into a battery's state, real-world battery operation during driving scenarios involves dynamic state changes, where current and voltage signals are far from ideally sinusoidal. To bridge the gap between EIS and real-world driving cycle analysis, we introduce the concept of a stochastic pulse design compatible with the load profile. This approach starts with frequency-based impedance data as a reference and transitions into time-based noisy permuted sinusoidal signals, eventually yielding stochastic pulse signals that more accurately reflect the complexities of real-world operation. The analysis of this multifaceted data is conducted in the latent space of an autoencoder, which comprises essential features extracted from the input data. Through latent space segmentation and its correlation with battery aging, we ensure the validity of the generated pulse signals compared to traditional EIS. Detailed point-to-point evaluations in the feature space enable the identification of the best and worst pulse load profiles, which can then be utilized to facilitate battery fast-charging and lifetime optimization.