TUT 1: Physics Meets Machine Learning (joint session DY/TUT/TT)

Machine learning has revolutionized many application fields such as computer vision and natural language processing. In physics there is a growing interest in using machine learning to enhance the analysis of experimental data and to devise and optimize experiments or numerical simulations. On the other hand physicists use their intuition and methods from statistical physics and complex systems theory to better understand the working principles of modern machine learning methods. This tutorial session introduces some subfields within this area and the basic methods involved.

Organized by Sabine Andergassen (Tübingen), Martin Gärttner (Heidelberg), Moritz Helias (Jülich), and Markus Schmitt (Cologne)

Time: Sunday 16:00–18:15 Location: HSZ 01

Tutorial TUT 1.1 Sun 16:00 HSZ 01

Machine Learning for Quantum Technologies — •Florian Marquardt — Max Planck Institute for the Science of Light and Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Machine learning is revolutionizing science and technology. In the past few years, it has become clear that it promises significant benefits as well for the development of quantum technologies. In this tutorial I will first give a brief introduction to neural networks. I will then discuss a number of areas and examples in which machine learning is being successfully applied in this context. These include measurement data analysis and quantum state representation, approximate quantum dynamics, parameter estimation, discovering strategies for hardware-level quantum control, the optimization of quantum circuits, and the discovery of quantum experiments, discrete quantum feedback strategies, and quantum error correction protocols.

Reference: "Artificial intelligence and machine learning for quantum technologies", M. Krenn, J. Landgraf, T. Foesel, and F. Marquardt, Phys. Rev. A 107, 010101 (2023).

Tutorial TUT 1.2 Sun 16:45 HSZ 01

The Unreasonable Effectiveness of Gaussians in the Theory of Deep Neural Networks — •Zohar Ringel — Racah Institute of Physics, Hebrew University in Jerusalem

Physical Sciences are in many ways the success story of explaining fundamental phenomena using simple math [1]. The fact that physical phenomena could be arranged in that manner is remarkable. Yet this simplicity does not necessarily carry over to life sciences or data sciences. Indeed prominent authors have argued against our desire to rely on neat mathematical structures when analyzing big data [2].

In the past half-decade several results have emerged which balance mathematical simplicity with data-induced complexity. These could be seen as a middle ground between the above juxtaposing views. The common divider here is the use of Gaussian distributions as approximants of various different quantities in deep neural networks (DNNs). Specifically these Gaussians emerge when describing outputs of DNNs with random weights, outputs of trained DNNs at random times, outputs of fixed DNNs over random input data, and fluctuations of hidden DNN pre-activations. In this tutorial I will present these quantities, provide arguments supporting their Gaussianity, and outline several theoretical implications.

[1] The Unreasonable Effectiveness of Mathematics in the Natural Sciences. Wigner (1960)

[2] The Unreasonable Effectiveness of Data. Halevy, Norvig, Pereira (2009)

Tutorial TUT 1.3 Sun 17:30 HSZ 01

Computing learning curves for large machine learning models using the replica approach — •Manfred Opper — Inst. für Softwaretechnik und Theor. Informatik, TU Berlin — Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, UK

Methods of statistical physics have been used for a long time to mathematically analyse the typical performance of machine learning models in the limit where both the number of data and the number of parameters (such as network weights) is large. By defining Boltzmann-Gibbs probability distributions over parameters where the cost function of the machine learning problem plays the role of a hamiltoninan, one can derive analytical expressions for training errors and generalisation errors using the corresponding partition functions and free energies in terms of a usually small number of order parameters.

Since the models depend on a set of random data to be learnt, additional appropriate statistical (so-called quenched) averages of free energies over this 'disorder' have to be performed. The replica approach is a prominent analytical tool from the statistical physics of disordered systems to solve this nontrivial technical challenge.

In this tutorial I will give an introduction to this approach. Starting with an explicit calculation for simple single layer perceptrons, I will then argue how the method can be applied to more complex problems such as kernel machines (support vector machines and Gaussian processes) and multilayer networks.

TUT 2: Stochastic Processes of Opinion Formation (joint session SOE/TUT)

Time: Sunday 16:00–18:15 Location: HSZ 02

Tutorial TUT 2.1 Sun 16:00 HSZ 02

Bounded Confidence Revisited: What We Overlooked, Underestimated, and Got Wrong — •Rainer Hegselmann — Frankfurt School of Finance & Management, 60322 Frankfurt, Adickesallee 32-34

The talk will discuss the so called bounded confidence model (BC-model, for short). The model is very simple: Period by period, all agents average over all opinions that are not further away from their actual opinion than a given distance Epsilon, their *bound of confidence*.

The simplicity of the model is deceptive. Two decades ago, Ulrich Krause and me published an analysis of the model in which we overlooked completely a decisive feature of our model: For increasing values of Epsilon, our analysis back then suggests smooth transitions in the model*s behavior. But in fact, the transitions are wild, chaotic, and non-monotonic.

In my talk I will present a new type of approach in which everything we overlooked at the time becomes directly obvious and, in a sense, unmissable. Key component of the new approach is an algorithm that identifies, exactly and exhaustively, all bounds of confidence, that make a difference. We get a list that, then, allows direct checks for wild behavior exhaustive of all possible cases. That is a good news. But it is accompanied by a bad one: The algorithm that does the work, requires an absolutely exact fractional arithmetic with integers of arbitrary length. As a consequence, we have to pay a price in terms of computational speed.

Tutorial TUT 2.2 Sun 16:45 HSZ 02

When intuition fails: the complex effects of assimilative and repulsive influence on opinion polarization — •Michael Maes[1], Andreas Flache[2], Shuo Liu[3], and Haoxiang Xia[3] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]University of Groningen, Groningen, The Netherlands — [3]Dalian University of Technology, Dalian, China

There is a debate about whether personalized services of social-media platforms contribute to the rise of bipolarization of political opinions. On the one hand, it is argued that personalized services of online social networks generate filter bubbles limiting contact between users who disagree. This reduces opportunities for assimilative social influence between users from different camps and prevents opinion convergence. On the other hand, empirical research also indicated that exposing users to content from the opposite political spectrum can activate the counter-part of assimilative influence, repulsive influence. Fostering contact that leads to opinion assimilation and limiting contacts likely to induce repulsive interactions, it has been concluded, may therefore prevent bipolarization. We demonstrate that these conclusions fail to capture the complexity that assimilative and repulsive influence generate in social networks. Sometimes, more assimilative influence can actually lead to more and not less opinion bipolarization. Likewise, increasing the exposure of users to like-minded individuals sometimes intensifies opinion polarization.

Tutorial TUT 2.3 Sun 17:30 HSZ 02

How growing connectivity and self-organization changes opinion dynamics — •Philipp Lorenz-Spreen — Center for Adaptive Rationality, Max Planck Institute for Human Development, Berlin, Germany

Information technology has made various aspects of our lives more dynamic and self-organized. Connections with others can be made across spatial and socio-demographic boundaries and undone with the click of a button. Since the famous six degrees of separation, networks seem much more connected; Facebook reports 3.5 degrees of separation on its friendship graph. Yet there have been repeated reports of segregated, homophilic network structures and related trends of increasing polarization on most online platforms. The mechanism that could resolve this apparent paradox may lie behind the question of whether we change our opinions according to our friends or whether we change our friends according to our opinions. We have recently proposed that an agent's opinion changes as a process of mutual reinforcement within clusters of shared attitudes and a coevolution of the associated network structure that dynamically adapts to changing opinions and follows a probability distribution governed by homophily. This combination helps explain the potential emergence of increasing polarization even as connectivity increases. Moreover, extending this model to multiple dimensions of topics can explain the empirical observation of increasing alignment of issues, where opinions become increasingly correlated within ideological clusters.

TUT 3: Hands-on tutorial on workflows for materials science simulation (joint session MM/TUT)

Time: Sunday 16:00–18:00 Location: HSZ 03

Tutorial TUT 3.1 Sun 16:00 HSZ 03

Hands-on tutorial on workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1], and Ralf Drautz[2] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf — [2]ICAMS, Ruhr-Universität Bochum

Advanced computational simulations in materials science have reached a maturity that allows one to accurately describe and predict materials properties and processes. The underlying simulation tasks often involve several different models and software that requires expert knowledge to set up a project and to vary input parameters. The accompanying increasing complexity of simulation protocols means that the workflow along the simulation chain becomes an integral part of research. Effective workflow management therefore is important for efficient research and transparent and reproducible results.

In this hands-on tutorial we will provide an interactive hands-on introduction into managing workflows with pyiron (www.pyiron.org). Pyiron is an integrated development environment for materials science built on python and Jupyter notebooks that may be used for a wide variety of simulation tasks, from rapid prototyping to high performance computing. The tutorial will first give a general introduction to using pyiron, with a focus on atomistic simulation tasks. In the second part of the tutorial, the training and validation of ace-machine learning potentials from reference density functional calculations will provide a real-life application example.

TUT 4: Strategic elements and sustainability (joint session MA/TUT)

Our appetite for resources is insatiable. The path to a climate-neutral society and economy requires the increasingly intensive use of strategy metals such as lithium, cobalt, nickel, but also the group of rare earth elements. This major transformation is not possible without the sustainable use of these so-called critical elements along the entire value chain. In the Tutorial "Strategic elements and sustainability", we have four eminent speakers looking in this context at new developments in batteries, catalysis, thermoelectrics and magnetism.

Organizers: Oliver Gutfleisch (TU Darmstadt) and Heiko Wende (U. Duisburg-Essen).

Time: Sunday 16:00–18:00 Location: HSZ 04

Invited Talk TUT 4.1 Sun 16:00 HSZ 04

Making better batteries? – From Li-ion to Na-ion batteries — •Philipp Adelhelm — Humboldt-University Berlin, Berlin, Germany — Helmholtz-Zentrum Berlin, Berlin, Germany

The shift to electromobility is one of the most important transformations currently taking place in our society. This is associated with a sharp increase in battery production, which on the one hand opens up new opportunities, but on the other hand also has a massive impact on raw material supply and supply chains. In addition, new large markets are emerging, such as stationary energy supply or mobile robotics. Lithium-ion batteries are currently the most attractive technology for this. However, due to the large demand for batteries and the different application scenarios, other technologies are also being pursued. Sodium ion batteries can be produced on the same production lines as lithium ion batteries and are therefore considered a "drop-in" technology. The aim here is to replace not only costly lithium but also other expensive elements such as nickel or copper. Work is therefore being done worldwide on a cell chemistry for sodium ion batteries that works almost as well as lithium ion technology, but at the same time is cheaper and more readily available, or has other specific advantages. The tutorial gives an introduction to sodium ion technology. The motivation and state-of-the art are explained in more detail and material aspects are discussed. In particular, the question is addressed which electrode materials are promising for sodium ion batteries, what is needed to achieve further progress and what actually happens when lithium ions are replaced by sodium ions in a battery.

Invited Talk TUT 4.2 Sun 16:30 HSZ 04

Sustainable Thermoelectric Materials Predicted by Data Mining and Machine Learning — •Kornelius Nielsch — Leibniz Institute of Solid States and Materials Research, Dresden, Germany — Institute of Materials Research at TU Dresden, Germany — Institute of Applied Physcis at TU Dresden, Germany

Generating electricity from temperature differences has proven itself in space. Thanks to this technology, the Voyager probes launched in 1977 are still sending signals today. In the meantime, the car industry and ship producers have become interested in thermoelectrics. The combustion of fossil fuels produces exhaust gas that is up to 1300 °C hot. Modern thermoelectric materials are continuously expanding the fields of thermoelectric applications. The experimental search for new thermoelectric materials remains largely restricted to a limited number of successful chemical and structural families, such as chalcogenides, skutterudites and zintl phases. In principle, computational tools such as density functional theory (DFT) offer the possibility of directing experimental synthesis efforts towards very different chemical structures. In practice, however, predicting thermoelectric properties based on first principles remains a difficult endeavour, and experimental researchers do not usually use computations directly to drive their own synthesis efforts. Strategies to bridge this practical gap between experimental requirements and computational tools will be discuss und presented in this tutorial talk. Ref: Energy Environ. Sci. 14, 3559 (2021) and Advanced Theory and Simulations 5, 2200351 (2022)

Invited Talk TUT 4.3 Sun 17:00 HSZ 04

Design strategies for electrocatalysts – an electrochemist's perspective — •Kristina Tschulik — Ruhr-Universität Bochum, Faculty for Chemistry and Biochemistry, Chair for Electrochemistry and Nanoscale Materials — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The aim to produce highly active, selective, and long-lived electrocatalysts by design drives major research efforts toward gaining fundamental understanding of the relationship between material properties and their catalytic performance. Surface characterization tools enable to assess atomic scale information on the complexity of electrocatalyst materials. Advancing electrochemical methodologies to adequately characterize such systems was less of a research focus point. In this tutorials, we shed light on the ability to gain fundamental insights into electrocatalysis and establish design strategies based on these. Concepts on how to improve mass transport, e.g. by exploiting magnetic fields are highlighted in this respect. Particular attention is paid to deriving design strategies for nanoelectrocatalysts, which is often impeded, as structural and physical material properties are buried in electrochemical data of whole electrodes. Thus, a second major approach focuses on overcoming this difference in the considered level of complexity by methods of single-entity electrochemistry. The gained understanding of intrinsic catalyst performance will ultimately allow us to advance design concepts to transforming "pre-catalysts" in the forseeable future.

Invited Talk TUT 4.4 Sun 17:30 HSZ 04

Green magnetic materials for efficient energy, transport and cooling applications — •Oliver Gutfleisch — TU Darmstadt, Material Science, Functional Materials

High performance hard and soft magnets are key components of energy-related technologies, such as direct drive wind turbines and e-mobility. They are also important in robotics and automatization, sensors, actuators, and information technology. The magnetocaloric effect (MCE) is the key for new and disruptive solid state-based refrigeration. Magnetic hysteresis and its inherent energy product characterise the performance of all magnetic materials. In the 60th position of the periodic table of elements is neodymium - an element that belongs to the rare earth-lanthanides and essential for the above applications. Basic material requirements, figure of merits, demand and supply, criticality of strategic elements and their recycling are explained for both permanent magnets and magnetocalorics referring to the benchmark materials NdFeB and LaFeSi. Every battery needs a magnet. 95% of electric vehicles utilize rare earth magnet-based drive motors, the quantities required global will grow from 5.000 t in 2019 to about 40.000 - 70.000 t per anno in 2030. The material history of neodymium is exciting and complex; monopolistic mining in China under ruinous conditions is just as problematic as our dependence on it. How "green" are the metals for renewable technologies? Who pays which price for it, and when?