Artificial intelligence, mathematics and physics

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CY Advanced Studies, Maison Internationale de la Recherche, CY Cergy-Paris Université

Organisers: A. Honecker (CY Cergy-Paris), R.A. Römer (Warwick)

Background and Purpose

Artificial intelligence and its incarnation as machine learning have matured to the level that researchers in fields such as Condensed Matter theory have during the past few years started to use the related tools in their ow research activities. First applications include the characterization of physical properties, such as identification of phases, as well as the determination of model parameters. In mathematics, there are questions about the framework behind machine learning and the characterization of the output of artificial intelligence. Further far-reaching consequences include ethical questions about the way how research is performed, and, in particular, ethical issues once human beings become a subject of such data-driven research themselves.

The purpose of this 2-day workshop is to bring together a broad panel of researchers from CY Cergy Paris Université with active interest in such questions, their international partners, notably from the University of Warwick and the MajuLab in Singapore, and a selection of both regional and international experts in the field in order to review the current status and to explore both scientific perspectives as well as potential future projects for collaboration.

Contents

Santiago Acevedo

Instituto de Fisica de La Plata, Buenos Aires, Argentina. CONICET

Phase diagram study of a 2D frustrated Ising antiferromagnet via unsupervised machine learning

We apply unsupervised learning techniques to classify the different phases of the J1-J2 antiferromagnetic Ising model on the honeycomb lattice [1]. We construct the phase diagram of the system using convolutional autoencoders. These neural networks can detect phase transitions in the system via anomaly detection [2] without the need for any label or a priori knowledge of the phases. We present different ways of training these autoencoders, and we evaluate them to discriminate between distinct magnetic phases. In this process, we highlight the case of high-temperature or even random training data. Finally, we analyze the capability of the autoencoder to detect the ground state degeneracy through the reconstruction error.

[1] S. Acevedo, M. Arlego, and C. A. Lamas. (2021), https://doi.org/10.1103/PhysRevB.103.134422

[2] Korbinian Kottmann, Patrick Huembeli, Maciej Lewenstein, and Antonio Acan. (2020), https://doi.org/10.1103/PhysRevLett.125.170603"

Connor Allen

University of Warwick

A Gaussian Approximation Potential for the TiAl system

A series of Gaussian approximation potentials (GAP) have been developed by training on density functional theory (DFT) predictions for free energy and derivative quantities for the TiAl system. The final GAP developed reproduced the underlying total energies with an average error below 1 meV (forces below 0.22eV/ Å). The average error in reproducing elastic constants for αTi, βTi, TiAl and Ti3Al was 7.45%, 12.6%,5.51%, and 23.2% respectively against DFT. The ordering of Al in αTi was also investigated through hybrid Monte Carlo molecular dynamics, and it was found that Al preferentially orders itself away from other Al nearest neighbours

Dr Albert Bartok-Partay

Department of Physics and School of Engineering, University of Warwick

Gaussian Approximation Potentials: fitting interatomic models from big data

In this talk I will discuss how microscopic observables available from first principles calculations, such as total energies and forces, can be used in combination with Gaussian Process regression to generate accurate interatomic models for a broad range of systems. I will introduce the tools and tricks that we discovered or invented along the way to make the scheme practical. In conclusion, I will present a few applications.

Ms Djenabou Bayo

Department of Physics, University of Warwick, Coventry, CV4 7AL, United Kingdom & CY Cergy Paris Universite, Laboratoire de Physique Theorique et Modelisation (LPTM) (CNRS UMR8089), 95302 Cergy-Pontoise, France

Machine learning the 2D percolation model

The percolation model is one of the simplest models in statistical physics displaying a phase transition. A classical lattice is occupied randomly with a given probability at each site (or bond). A phase transition from a non-percolating to a percolating state appears around a probability pc, the so-called percolation threshold. Machine Learning (ML) and Deep Learning (DL) techniques are still relatively new methods when applied to physics. Recent work shows that ML/DL techniques allow to detect phase transitions directly from images of computed quantum states. Here, we implement ML/DL techniques to identify the percolation threshold in 2D by identifying the connectivity properties of percolation clusters. We employ a standard image classification strategy with a multi-layered convolutional neural network. In addition, we also work directly with the numerical raw data. The implementation is carried out in Python with the ML/DL libraries of Pytorch. We pay special attention to the question of whether these DL methods can indeed identify percolation, i.e., spanning clusters, or are just counting occupation densities.

Nils Caci

RWTH Aachen University

Critical phenomena in anisotropic S=1 Heisenberg antiferromagnets on the honeycomb lattice

We consider two-dimensional spin-1 antiferromagnets with distinct single-ion anisotropies along two perpendicular axes. For a single easy-plane anisotropy, a Berezinsky-Kosterlitz-Thouless (BKT) transition is known to appear, below which quasi long-range order emerges. Instead, in the case of different anisotropies along two perpendicular axes a thermal Ising transition with (true) long-range magnetic order appears. Recent inelastic neutron scattering experiments on the compound BaNi2V2O8 indicate that near to the critical point reminiscent BKT scaling still prevails. We investigate this scenario by means of large-scale quantum Monte-Carlo simulations.

Burak Civitcioglu

LPTM, CY Cergy-Paris Université, France

Machine Learning Methods applied to the 2D Ising Model

The Ising model is one of the most studied models in statistical physics. It is well known to exhibit an ordering transition in two dimensions (2D). Snapshots of magnetic configurations taken above and below the phase transition show clear differences in the distribution of spins. Recently, machine learning methods have been shown to be successful in identifying and classifying such differences across many types of images, and also to the 2D Ising model. Here, we study the performance and the limits of such classification models and move onto the regression models. In particular, we investigate how accurately the temperature of a given configuration can be classified from just the image, and then show that in fact the regression model to predict the energies instead of temperatures give significantly better results. We use the TensorFlow environment as the main machine-learning environment and train with various neural network architectures.

Dr Mats Granath
Department of Physics, University of Gothenburg, Sweden

Deep machine learning applied to topological stabilizer codes and topological band structures

Topological order is a major theme in condensed matter physics, with potential applications to novel classical computers as well as quantum computers. We apply deep machine learning techniques to two different problems related to topological order: 1) To build error protected quantum computers, topological stabilizer codes, such as Kitaev's toric code, is currently seen as the most promising approach to quantum error correction. Decoding the syndrome, which provides information about the configuration of errors in such a quantum code, is a computationally demanding task. We have applied deep reinforcement learning to the decoding problem and show that an AI agent can be trained to perform error correction with an accuracy which is higher than standard heuristic decoders [1,2]. 2) In a different project [3,4] we develop an unsupervised deep learning method, Topological data augmentation, to classify topological band structures according to topological index. By designing neural networks in an informed way, it is found that the networks can actually learn to calculate the appropriate momentum space local quantities to find the aggregate topological index, which allows for interpretable classifiers that generalize beyond the training data.

1. P. Andreason et al. Quantum 3,183 (2019)

2. D. Fitzek et al. Phys. Rev. Res. 2, 023230 (2020)

3. O. Balabanov and M.G. Phys. Rev. Res. 2, 013354 (2020)

4. O. Balabanov and M.G. Machine Learning: Sci. and Tech. 2, 025008 (2020)

Nistor Govrazu
ETIS, CYU Cergy-Paris

Unsupervised Collaborative Machine Learning: Methods and Applications

Transfer and collaborative learning allows the transfer/collaboration of models by transferring the knowledge from one source to another. Within the framework of collaborative clustering and depending on the structure of collaborative datasets, there are three main types of collaboration: horizontal, vertical and hybrid. In these works, I am particularly interested in horizontal collaboration where groups of data are described in different spaces: each dataset is described by different attributes, but has the same individuals as the other datasets (views in a multi-view framework). The problem is: how to make clustering from a collection of distributed classifications from different features space? For this type of problem, the validation of the collaboration results becomes difficult, because all the partitionings are 'correct' but obtained with different representations. I propose several models to address this problem using topological learning, learning based on non-negative matrix factorization, and probabilistic models. These models have been validated theoretically and experimentally on different types of data: numerical, text, images, graphs. This work opens new perspectives for learning multi-source and heterogeneous data and can be adapted in a quantum artificial learning framework.

Prof. Nicholas Hine

University of Warwick

Machine Learned Interatomic Potentials for Theoretical Spectroscopy of Molecules in Solvent Environments

Accurate simulations of the excited state dynamics of chromophores in complex environments are a prerequisite to understanding important properties such as photostability, relaxation pathways, and excited state lifetimes. An atomistic understanding of these properties can aid in the design and study of useful chemical compounds such as novel sunscreen candidates. However, with an explicit representation of the solvent, there are conflicting requirements set by the need to follow individual trajectories over long timescales, to sample over the ensemble of solvent configurations, and to use a high level of theory to obtain good chemical accuracy, which means these timescales are not accessible with DFT or QC methods alone. A commonly-used approach is to sample from the dynamics of a lower level of theory and then perform higher-level calculations on extracted clusters: however, excitation energies are very sensitive to atomic positions and this results in notable inaccuracy. Our new approach uses machine learning to approximate ground and excited state potential energy surfaces of full explicit models of chromophores in a variety of solvent environments. This allows for an acceleration of the dynamics simulations, while retaining the accuracy of DFT or higher level methods. Our workflow is based in ESTEEM: Explicit Solvent Toolkit for Electronic Excitations of Molecules [1]. Building on the ASE framework, ESTEEM can call on a range of different electronic structure, molecular dynamics, and machine learning codes, to calculate excited state and spectroscopic properties of molecules in solvent environments. [1] https://esteem.readthedocs.io/en/latest/

Prof Michael Hilke

McGill University and University of Florence (2021-2022)

Quantum enhanced machine learning for Covid-19 and Anderson metal-insulator predictions

After introducing quantum machine learning, we discuss the implementation of a quantum learning algorithm on a quantum computer and a quantum simulator. We use US Covid-19 data to predict safe and unsafe regions using our quantum learning algorithm. This algorithm is then applied to evaluate the phase boundary of the 3D metal-insulator transition using simulated data. We compare the quantum algorithm with classical analogues and find that in most cases the classical ones outperform the quantum ones with some exceptions that we discuss in more detail.

Dr Katarina Karlova

P. J. Safarik University in Kosice, Slovakia

Localized-magnon approach for spin-1/2 Heisenberg diamond-like decorated square lattice

This work is devoted to a theoretical examination of a frustrated quantum Heisenberg spin model on two-dimensional diamond-like decorated square lattice, which will be treated by making use of two complementary methods known as the localized-magnon theory and density-matrix renormalization group simulations. The localized-magnon approach will be developed in order to investigate the ground-state and low-temperature magnetic properties in a highly frustrated parameter region, while the density-matrix renormalization group simulations will be contrarily used in order to

construct numerically exact ground-state phase diagram. This combined study will thus provide a more comprehensive understanding of all remarkable quantum features of the Heisenberg model on diamond-like decorated lattices in a highly frustrated region. In particular, our attention will be focused on low-temperature thermodynamics and magnetization process in a highly frustrated region. In addition, it will be shown that the investigated quantum spin model turns out to be useful for low-temperature refrigeration achieved by the process of adiabatic demagnetization.

Prof Dmitry Kovrizhin

LPTM, CY Universite Cergy-Paris, France

Topological electrostatics

We present a theory of optimal topological textures in nonlinear sigma-models with degrees of freedom living in the Grassmannian Gr(M,N) manifold. These textures describe skyrmion lattices of N-component fermions in a quantising magnetic field, relevant to the physics of graphene, bilayer and other multicomponent quantum Hall systems near integer filling factors v>1. We derive analytically the optimality condition, minimizing topological charge density fluctuations, for a general Grassmannian sigma model Gr(M,N) on a sphere and a torus, together with counting arguments which show that for any filling factor and number of components there is a critical value of topological charge above which there are no optimal textures. Below this critical value the solution of the optimality condition on a torus is unique, while in the case of a sphere one has, in general, a continuum of solutions corresponding to new {\it non-Goldstone} zero modes, whose degeneracy is not lifted (via order from disorder mechanism) by any fermion interactions depending only on the distance on a sphere. We supplement our general theoretical considerations with the exact analytical results for the case of Gr(2,4), appropriate for recent experiments in graphene.

Prof Carlos Alberto Lamas

CONICET - Institute of Physics La Plata, UNLP

XiaoLong Liu

Xiangtan University, Xiangtan

Jie Liu

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Prof Elisabeth Logak

Math Dpt, CYU

Prof Robert MacKay

Mathematics, University of Warwick

Artificial intelligence optimisation may lead to unethical solutions

(with H.Battey, N.Beale, A. Davison)

In a classic piece of journalism published by the Sun (22 Jan 2018), B. Leo tried out several reputable online car-insurance sites; he found that changing the client's first name from John to Mo increased the quotes by 11-69%. This is considered by most people to be unethical; more pragmatically it risks

liability for compensation or fines, business-loss and employee-disaffection. Nowadays, most online sites are committed to name-independent processing, but personal information is remarkably easy to determine from relatively little data.

We show that if the distribution of profits from a "red" set of strategies has higher mean than from a "green" set then an optimising AI is overwhelmingly likely to choose a red strategy. We compute the asymptotics of the "unethical odds ratio" Y of the optimal strategy in a large number of trials, using extreme value theory.

The work suggests that even if the AI knows legal and ethical constraints, it could be important to have a human check what it is choosing.

Reference: N Beale, H Battey, AC Davison, RS MacKay, An unethical optimization principle, RSOS 7 (2020) 200462

Prof Angus MacKinnon
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Peter Mühlbacher
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Prof Arlego Marcelo
Instituto de Fisica La Plata (IFLP), La Plata, Buenos Aires, Argentina

Dr Hui Khoon Ng
Yale-NUS College, and the Centre for Quantum Technologies, National University of Singapore

Adaptive quantum state tomography with neural networks

Current algorithms for quantum state tomography (QST) are costly both on the experimental front, requiring measurement of many copies of the state, and on the classical computational front, needing a long time to analyze the gathered data. Here, we introduce neural adaptive quantum state tomography (NAQT), a fast, flexible machine-learning-based algorithm for QST that adapts measurements and provides orders of magnitude faster processing while retaining state-of-the-art reconstruction accuracy. As in other adaptive QST schemes, measurement adaptation makes use of the information gathered from previous measured copies of the state to perform a targeted sensing of the next copy, maximizing the information gathered from that next copy. Our NAQT approach allows for a rapid and seamless integration of measurement adaptation and statistical inference, using a neural-network replacement of the standard Bayes' update, to obtain the best estimate of the state. Our algorithm, which falls into the machine learning subfield of "meta-learning" (in effect "learning to learn" about quantum states), does not require any ansatz about the form of the state to be estimated. Despite this generality, it can be retrained within hours on a single laptop for a two-qubit situation, which suggests a feasible time-cost when extended to larger systems and potential speed-ups if provided with additional structure, such as a state ansatz. [Reference: Y Quek, S Fort, and HK Ng, npj Quantum Information 7, 105 (2021).]

Prof Tomi Ohtsuki

Physics Division, Sophia University

Machine learning magneto-fingerprints

In collaboration with K. Tsunekawa, S. Daimon, S. Kawakami, T. Kikkawa, R. Ramos, K. Oyanagi, and E. Saitoh

At very low temperature, the electric conductance of a nano-sized semiconductor exhibits complex but reproducible patterns as a function of magnetic fields, which is called quantum fingerprints or magneto-fingerprints. They originate from quantum interference of electrons. Although the interference patterns are considered to reflect microscopic information of scattering, they are too complicated for human to understand. Here we show that neural network-based machine learning allows us to decipher magneto-fingerprints; from a magneto-fingerprint, we predict the spatial images of electron wave functions in a sample. The output wave function image reveals quantum interference of conduction electrons as well as the positions of scatterers. Thus, by measuring the magneto-conductance we can obtain the positions of scatterers inside the sample without relying on the microscopes.

Dr Jozef Strecka

P. J. Safarik University in Kosice, Slovakia

Spin-1/2 Heisenberg diamond and octahedral chains as a statistical-mechanical problem of hard-core monomers and dimers

Ground-state phase diagram of quantum spin-1/2 Heisenberg diamond and octahedral chains is elaborated from a mapping correspondence with effective mixed-spin Heisenberg chains, which are derived by employing a local conservation of a total spin on vertical dimers of a diamond chain and square plaquettes of an octahedral chain, respectively. It has been recently demonstrated that the lowest-energy eigenstates of the spin-1/2 Heisenberg diamond [1] and octahedral [2,3] chains follow in a highly-frustrated parameter region from flat bands, which correspond to magnons bound on vertical dimers of diamond chain and square plaquettes of octahedral chain, respectively. This fact allows a precise description of low-temperature thermodynamics above the monomer-dimer and monomer-tetramer ground states of the spin-1/2 Heisenberg diamond and octahedral chains from a mapping correspondence with a classical one-dimensional lattice-gas model of hard-core monomers. In the present work we will adapt the localized-magnon approach to a less frustrated parameter region supporting more peculiar dimer-tetramer and tetramer-hexamer ground states of the spin-1/2 Heisenberg diamond and octahedral chains with a spontaneously broken symmetry. It will be verified by a direct comparison between exact diagonalization and localized-magnon approach that the low-temperature thermodynamics above the dimer-tetramer and tetramer-hexamer ground states of the spin-1/2 Heisenberg diamond and octahedral chain can be satisfactorily described by a classical lattice-gas model of hard-core monomers and dimers.

[1] O. Derzhko, J. Richter, O. Krupnitska, Condens. Matter Phys. 15 (2012) 43702.

[2] J. Strecka, J. Richter, O. Derzhko, T. Verkholyak, K. Karlova, Phys. Rev. B 95 (2017) 224415.

[3] J. Strecka, J. Richter, O. Derzhko, T. Verkholyak, K. Karlova, Physica B 536 (2018) 364-368.

Prof. Guy Trambly de Laissardière

LPTM, CY Cergy Paris Universite, France

Electronic flat-bands in 2D materials

- Magnetism in bilayer twisted graphene (with and without strain), MoS2 (preliminary results) and transport in bilayer graphene

- Transport of flat bands due to defects in AB graphene bilayers

- Properties of the flat-bands of edge states

Cecilia Tarpau

CY Cergy Paris Universite, France

Data-driven approaches for correcting artefacts on Compton scattered tomographic images

Computed Tomography (CT) is one of the privileged imaging techniques to explore matter today and its internal structure without destroying it. Classical CT uses only primary radiation, that is, transmitted radiation without any deviation, from the source to the detector. However, when passing though matter, a significant proportion of photons may be scattered by the Compton effect. As a consequence, Compton scattering is the cause of serious degradation in the quality of reconstruction, in terms of blurring and loss of contrast. This may lead to false detection and influence the conclusions of diagnoses. On the other hand, Compton scattered radiation can also be considered as a useful and significant part of information, which can also be used for tomographic reconstruction. This observation is the starting point of the development of imaging systems of Compton Scattering Tomography (CST).

We introduced two CST configurations during my thesis. The first one, called Circular CST (CCST), consists of a fixed source and a ring of detectors passing through the source [2,3]. The studied CST configuration is made of a fixed source and a detector rotating around the source [4]. For each CST system, we modelled data acquisition and proposed an algorithm for image reconstruction. Both simulation results from the proposed algorithms revealed a common and general problem about quality of reconstruction. In fact, even if the obtained results give a good representation of the object under study (with a sufficient resolution and contrast, a good distinction of internal details of the object), reconstructions exhibit artefacts. Even if these artefacts are well explained theoretically, it is difficult to reduce them without increasing drastically the calculation time of reconstruction. My recent research work consists in studying how machine learning can help us in this task. I will present the first obtained results.

[1] A. M. Cormack, Journal of Applied Physics, vol. 34, no. 9, pp. 2722–2727, 1963.
[2] C. Tarpau et. al, IEEE Trans. Radiation and Plasma Medical Sciences, vol. 4, no. 4, pp. 433-440, 2020.
[3] C. Tarpau et. al, Journal of Electronic Imaging, vol. 29, no. 1, 2020.
[4] C. Tarpau et. al, IEEE Trans. Computational Imaging, vol. 6, pp. 958-967, 2020.

Prof Giorgos Tsironis

Department of Physics and Institute for Theoretical and Computational Physics, University of Crete, Greece

Discovering nonlinear resonances through physics-inspired machine learning

For an ensemble of nonlinear systems that model, for instance, molecules or photonic systems, we propose a method that finds efficiently the configuration that has prescribed transfer properties. Specifically, we use physics- informed machine learning (PIML) techniques to find the parameters for the efficient transfer of an electron (or photon) to a targeted state in a nonlinear dimer. We create a machine learning model containing two variables that represent the nonlinear terms in a donor-acceptor system. Subsequently we introduce a data-free physics-inspired loss function as 1.0 – P(j) , where P(j) is the probability, the electron being in the targeted state,. By minimizing the loss function, we maximize the occupation probability to the targeted state j. The method recovers known results in the targeted energy transfer (TET) nonlinear model, and it is then applied to a more complex system with an additional intermediate state. In this trimer configuration, the PIML approach discovers desired resonant paths from the donor to acceptor units. The proposed PIML method is general and may be used in the chemical design of molecular complexes or engineering design of quantum or photonic systems.

Prof Daniel Ueltschi

Mathematics, Warwick

Loop models and the universal distribution of the loop lengths

Loop models involve one-dimensional loops living in the 3D space. They appear as representations of several models in Statistical Physics, such as classical and quantum spin systems, bosonic systems, field theories. I will argue that the joint distribution of the lengths of long loops, in all loop models, is given by a Poisson-Dirichlet distribution. The explanation involves a Glauber dynamics where the loops satisfy an effective mean-field split-merge process, whose invariant measure is Poisson-Dirichlet.

Dr Ozgun YILMAZ

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