Workshop on Classical and Quantum Machine Learning for Condensed Matter Physics | (SMR 3948)

19 Jun 2024 - 21 Jun 2024
Virtual

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T01

Phase classification in disordered quantum systems through machine learning

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This talk discusses the use of supervised machine learning to explore phase transitions in the long-range Aubry-André Harper (LRH) model, a one-dimensional quasiperiodic system[1]. By training a neural network on eigenstates, we identify delocalized, localized, and multifractal phases. When applied to the Aubry-André Harper (AAH) model, the neural network accurately maps the phase diagram, with results aligning with traditional fractal dimension analysis. Furthermore, binary classification based on probability density enables the identification of critical transition points. The findings suggest that neural networks are a powerful tool for identifing phase transitions in condensed matter physics.

[1] **A. Ahmed***, A. Nelson*, A. Raina and A. Sharma, Phase classification in the long-range Harper model using machine learning, Phys. Rev. B 108, 155128 (2023)
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T02

MatFeaLib: Materials Features Library Python Package

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Materials representations play a crucial role in the development of successful machine learning models for the prediction of materials properties [1]. These representations aim to map materials samples into proper feature spaces for machine learning approaches. Chemical composition can be encoded in terms of different atomic features, such as electronic, thermodynamic, and periodic table characteristics of individual elements. MatFeaLib (Materials Features Library) is a Python package designed to easily generate atomic representations for use in machine learning algorithms. This library offers distinct functions for generating atomic feature vectors and corresponding statistical quantities and is able to deal with the input compounds in the form of a string, a list, or a Pandas DataFrame.
MatFeaLib covers various internal atomic features collected from different sources, including DFT features obtained within PBE or HSE functionals, atomic features from the Mendeleev package [2], and atomic features from reference [3]. The complete list of collections can be accessed from package documentation [4]. Each of these collections contains a different set of atomic features that can be chosen arbitrarily. The statistical derivatives of atomic features, implemented via NumPy [5] and SciPy [6] packages, are useful for the description of multi-stoichiometric material data [7]. Users can select their desired statistical quantities as a string or a list. The supported functions include sum, standard deviations, skewness, and entropy. The output of MatFeaLib is in a proper DataFrame format for various machine learning packages including Scikit-learn [8].

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T03

Abstract template for Classical and Quantum Machine Learning for Condensed Matter Physics | Smr (3948)

Resolving degeneracies in Google search via quantum stochastic walks

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The internet is one of the most valuable technologies invented to date. Among them, Google is the most widely used search engine. The PageRank algorithm is the backbone of Google search, ranking web pages according to relevance and recency. We employ quantum stochastic walks (QSW) with the hope of bettering the classical PageRank (CPR) algorithm, which is based on classical continuous time random walks (CTRW). We implement QSW via two schemes: only incoherence and dephasing with incoherence. PageRank using QSW with only incoherence or QSW with dephasing and incoherence best resolves degeneracies that are unresolvable via CPR and with a convergence time comparable to that for CPR, which is generally the minimum. For some networks, the two QSW schemes obtain a convergence time lower than CPR and an almost degeneracy-free ranking compared to CPR.

The talk will be based on the published article [1].

[1] Journal of Statistical Mechanics: Theory and Experiment (2024) 013402.

T04

Abstract template for Workshop on Classical and Quantum Machine Learning for Condensed Matter Physics

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We present the quantum simulation of the frustrated quantum spin-$\frac{1}{2}$ antiferromagnetic Heisenberg spin chain with competing nearest-neighbor (J_1) and next-nearest-neighbor (J_2) exchange interactions in the real superconducting quantum computer with qubits ranging up to 100. In particular, we implement, for the first time, the Hamiltonian with the next-nearest neighbor exchange interaction in conjunction with the nearest neighbor interaction on IBM's superconducting quantum computer and carry out the time evolution of the spin chain by employing the first-order Trotterization. Furthermore, our novel implementation of the second-order Trotterization for the isotropic Heisenberg spin chain, involving only nearest-neighbor exchange interaction, enables precise measurement of the expectation values of staggered magnetization observable across a range of up to 100 qubits. Notably, in both cases, our approach results in a constant circuit depth in each Trotter step, independent of the number of qubits. Our demonstration of the accurate measurement of expectation values for the large-scale quantum system using superconducting quantum computers designates the quantum utility of these devices for investigating various properties of many-body quantum systems. This will be a stepping stone to achieving the quantum advantage over classical ones in simulating quantum systems before the fault tolerance quantum era.

[1] T. A. Chowdhury, K. Yu, M. A. Shamim, M. L. Kabir and R. S. Sufian, "Enhancing quantum utility: simulating large-scale quantum spin chains on superconducting quantum computers," [arXiv:2312.12427 [quant-ph]].

T05

Differentiable Monte Carlo for spin models

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Spin models are mathematical representations of spins, which can symbolize various physical entities such as magnetic moments, lattice sites, and biological cells. One of the most extensively studied spin systems is the Ising model, where each spin can take on one of two values. Typically, spins interact locally with their nearest neighbors. Despite its simplicity, the Ising model exhibits intriguing phenomena such as criticality, where a phase transition can occur depending on the lattice configuration and external physical parameters, such as temperature and magnetic field.

To study the behavior of spin models, simulations are essential. Due to the complexity of analyzing these systems analytically, numerical methods become necessary. One such technique is the Monte Carlo method, which simulates spin models by sampling possible spin configurations and transitioning to states of higher probability. This approach allows for the investigation of the physical properties of spin models.

Beyond simulating magnetic systems, spin models have versatile applications across various fields. In biology, they are used to study the behavior and interactions of biological cells, providing insights into complex cellular processes and structures. In the realm of machine learning, spin models contribute to the development of algorithms by helping to optimize configurations and solve complex optimization problems. Additionally, in combinatorial problems, spin models are employed to find solutions for logistical challenges by exploring numerous possible configurations and selecting the most optimal outcomes. This interdisciplinary utility underscores the importance of spin models in both theoretical research and practical applications.

In this work, we introduce a modification to the Monte Carlo method that renders the technique differentiable [1]. This advancement enables the optimization of a spin system with respect to its properties, such as the exchange interaction or the spin values themselves. By making the Monte Carlo method differentiable, we can apply gradient-based optimization techniques to fine-tune the system's parameters, thereby enabling the Monte Carlo method as a machine learning technique.

We demonstrate the efficacy of this method by applying it to two distinct optimization problems. The first application involves optimizing the spin interactions to achieve a desired spin configuration, even in the presence of thermal fluctuations. The second application focuses on finding the ground state of the system by guiding the Monte Carlo simulation using gradient information.

Differentiable Monte Carlo has the potential to be applied to a variety of systems and problems. By combining Monte Carlo with optimization techniques, we can significantly extend its capabilities, particularly in the realm of machine learning. This integration opens up new avenues for utilizing Monte Carlo methods to solve complex optimization tasks, enhance model performance, and contribute to advancements in various scientific and engineering domains.

[1] Farias, Tiago S., et al. "A Differentiable Programming Framework for Spin Models." Computer Physics Communications, vol. 302, Sept. 2024, p. 109234. ScienceDirect, https://doi.org/10.1016/j.cpc.2024.109234.

T06

Abstract template for Workshop on Classical and Quantum Machine Learning for Condensed Matter Physics

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Photonic topological states play an important role in recent optical physics and has led to the design of devices with robust properties [1]. The topological properties in photonic systems relate to several optical phenomena. In one-dimensional systems, for instance, this topological property is called Zak phase [2] and it can be used to predict the existence of topological interface states [3] which indeed are states characterized by their robustness to certain type of perturbation and disorder in the system. The works about topological photonics reported to date are mostly based on a forward-design approach where first we precisely define the geometric parameters and subsequently obtain the wave response such as wave dispersion/frequency response. In this process, a set of geometric entities are supplied and wave response is calculated. But what is even more interesting is the inverse design problem, meaning the direct retrieval of the proper structure for the desired optical performance, which traditionally seems infeasible as it requires exploration of a much larger degree of freedom in the design space, and hence is more challenging. However recently, deep learning (DL), a subset of machine learning that learns multilevel abstraction of data using hierarchically structured layers, offers an efficient means to design photonic structures and also it was proved to be very efficient in solving the inverse design problem [4], for instance, Inverse design models based on DL used to predict the topological properties of 1D photonic [5,6], specifically through the prediction of the Zak phase. In this work a data-driven DL model is devloped to inversely design a topological photonic system with targeted topological property. Our focus here is on the Zak phase, which is the topological property of one-dimensional photonic crystals. After learning the mapping between the geometrical parameters and the Zak phases, the neural network can be used to obtain the appropriate photonic structures by applying the objective Zak phase properties. Our work would give more insights into the application of deep learning on the inverse design of the complex photonic systems.

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[5] L. Yang, R. Jie, et al, Appl. Phys. Lett. **114**, (2019)
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T07

Machine learning prediction of thermal and elastic properties of double half-Heusler alloys

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Double half-Heusler alloys are promising materials for applications as magnetocaloric materials, topological insulators, but especially thermoelectric materials. Four different elements in their composition provide a wide range of possible compositions, which, on the other hand, is difficult to study directly by applying traditional first-principles approaches to large number of compositions. In this work [1], based on the gradient boosting method, regression models are constructed that allow rapid prediction of the lattice thermal conductivity, as well as a number of other thermal and elastic properties, based on the composition and crystal structure of a compound. This made it possible for the first time to calculate the lattice thermal conductivity, as well as Grüneisen parameter, Debye temperature, and elastic moduli for a number of double half-Heusler compounds. We observe that the predicted thermal conductivity is in better agreement with the experimental data than the results of density functional theory calculations available in the literature. As a result, we have predicted a number of stable double half-Heusler compounds with thermal conductivity lower than previously known in this class of compounds. In addition, the importance of various features for predicting each of the studied properties, and the effect of the crystallographic symmetry of the compound on the prediction accuracy were analysed. This study was supported by the grant of RSF No 22-22-20109.

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T08

Abstract template for Workshop on Classical and Quantum Machine Learning for Condensed Matter Physics

Supervised and unsupervised machine learning techniques applied to skyrmion systems

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Machine learning (ML) techniques have certainly gained significant interest in the last few years in every area of scientific research, including condensed matter physics. Among the many areas where ML has been applied are a variety of complex topological spin systems, such as skyrmions, swirling magnetic textures characterized by a topological charge that renders them stable agaisnt perturbations, and thus relevant for future computational applications. ML has been used to classify stable phases in a typical skyrmion phase diagram (helices, skyrmion crystals and ferromagnetic) [1,2], extract information from interactions [3] and predict order parameters [4].

Here, we discuss two machine learning approaches to explore skyrmion phase diagrams. Firstly, we present a classification approach to determine intermediate phases (bimerons and skyrmion gas) that are enhanced with temperature in snapshots obtained from simulations of a typical skyrmion model that combines ferromagnetic exchange and in-plane Dzyaloshinskii Moriya interactions [2]. We train and validate a Convolutional Neural Network (CNN), a technique that is known to work very well on images, and apply it to an independent training set (snapshots from models with different DM), with surprising results. We compare these CNN results to those obtained with other ML classification algorithms, Support Vector Machine and Decision Trees.

Secondly, we resort to the 'anomaly detection' technique, an unsupervised ML technique that aims to detect data that is 'different' from the rest. Our main goal here is to detect exotic phases in skyrmion phase diagrams. To do this, we train a Convolutional Autoencoder (CAE) with a set of skyrmion crystal snapshots obtained from a parametrisation, and then apply it to snapshots from Monte Carlo simulations of different models for a wide range of temperature and magnetic fields [5]. We calculate the root mean square error (RMSE) between the original image and the output obtained after applying the trained CAE. We find that the RMSE may be useful to not only detect exotic low temperature phases, but also to distinguish between the characteristic low temperature orderings of a skyrmion system.

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[5] F. A. Gómez Albarracín arXiv:2404.10943

T09

Approximately-symmetric neural networks for quantum spin liquids

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We propose and analyze a family of approximately-symmetric neural networks for quantum spin liquid problems [1]. These tailored architectures are parameter-efficient, scalable, and significantly outperform existing symmetry-unaware neural network architectures. Utilizing the mixed-field toric code model, we demonstrate that our approach is competitive with the state-of-the-art tensor network and quantum Monte Carlo methods. Moreover, at the largest system sizes (N = 480), our method allows us to explore Hamiltonians with sign problems beyond the reach of both quantum Monte Carlo and finite-size matrix-product states. The network comprises an exactly symmetric block following a non-symmetric block, which we argue learns a transformation of the ground state analogous to quasiadiabatic continuation of Hastings&Wen [2]. Our work paves the way toward investigating quantum spin liquid problems within interpretable neural network architectures.

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T10

THE IMPACT OF WEAK MEASUREMENTS ON EXCITON-EXCITON INTERACTIOS

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In our study of super quantum discord between two excitonic qubits inside a coupled semiconductor quantum dots system, our primary focus is to uncover the impact of weak measurement on its quantum characteristics. To achieve this, we analyze how varying the measurement strength x, affects this super quantum correlation in the presence of thermal effects. Additionally, we assess the effect of this variation on the system's evolution against its associated quantum parameters; external electric fields, exciton-exciton dipole interaction energy and Förster interaction. Our findings indicate that adjusting x to smaller values effectively enhances super quantum correlation, making weak measurements act as a catalyst. This adjustment ensures its robustness against thermal effects while preserving the non-classical attributes of system. Furthermore, our study unveils that the effect of weak measurements on this latter surpasses the quantum effects associated with the system. Indeed, manipulating the parameter x allows weak measurement to function as a versatile tool for modulating quantum characteristics and controlling exciton-exciton interactions within the coupled semiconductor quantum dots system.