KITS Workshop

Machine Learning and Many-Body Physics

Kavli Institute for Theoretical Sciences (KITS), UCAS
http://ml2017.csp.escience.cn

Jun. 28 – Jul. 7, 2017
University of Chinese Academy of Sciences
No. 3 Zhong-Guan-Cun Nan-Yi-Tiao Road, Haidian Dis.
Beijing, China

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Contributors

Workshop Program

Tutorials (S101, Blackboard talks in S102)

Jun. 28 (Wed.)		
10:00-11:30	**Wei-Shan Dong** Baidu Research	A Brief Introduction to Machine Learning
11:30-14:00	*Lunch*	
14:00-15:30	**Matthias Rupp** FHI Berlin	[Blackboard] Machine Learning for Quantum Mechanics
15:30-16:00	*Break*	
16:00-17:30	**Juan Carrasquilla** D-Wave System	Machine Learning Phases of Matter
Jun. 29 (Thur.)		
10:00-11:30	**Xun Gao** Tsinghua IIIS	[Blackboard] Quantum Machine Learning
11:30-14:00	*Lunch*	
14:00-15:30	**Hai-Jun Zhou** ITP, CAS	[Blackboard] Message Passing for Graphical Models
15:30-16:00	*Break*	
16:00-17:30	**Giuseppe Carleo** ETH Zurich	[Blackboard] Neural Network Quantum States
Jun. 30 (Fri.)		
10:00-11:30	**Yang Qi** MIT	Guiding Monte Carlo Simulations with Machine Learning
11:30-14:00	Lunch	
14:00-15:30	**Miles Stoudenmire** UC Irvine	[Blackboard] Tensor Network States and Algorithms
15:30-16:00	Break	
16:00-17:30	**Yi-Zhuang You** Harvard	Machine Learning and Tensor Network Holography

Conference (S101)

Jul. 3 (Mon.)		
09:00-09:15	**Fu-Chun Zhang** KITS, UCAS	Welcome and Opening
09:15-10:00	**Giuseppe Carleo** ETH Zurich	Neural-network Quantum States
10:00-10:45	**Masatoshi Imada** Univ. of Tokyo	Simulating quantum many body problems of fermions and quantum spins
10:45-11:15	*Break*	
11:15-12:00	**Xun Gao** Tsinghua IIIS	Efficient Representation of Quantum Many-body States with Deep Neural Networks
12:00-14:00	*Lunch*	
14:00-14:45	**Juan Carrasquilla** D-Wave System	A neural network perspective on the Ising gauge theory and the toric code
14:45-15:30	**Ye-Hua Liu** ETH Zurich	Learning Phase Transitions with/without Confusion
15:30-16:00	*Break*	
16:00-16:45	**Frank Yi Zhang** Cornell Univ.	Quantum Loop Topography for Machine learning-on topological phase, phase transitions, and beyond
16:45-17:30	**Ehsan Khatami** San Jose State Univ.	Machine learning phases of strongly-correlated fermions
Jul. 4 (Tue.)		
09:00-09:45	**Masayuki Ohzeki** Tohoku Univ.	Sparse modeling: how to solve the ill-posed problem
09:45-10:30	**Junya Otsuki** Tohoku Univ.	Sparse modeling approach to analytical continuation and compression of imaginary-time quantum Monte Carlo data
10:30-11:00	*Break*	
11:00-11:45	**Richard Scalettar** UC Davis	Magnetic Phase Transitions and Unsupervised Machine Learning
11:45-12:15	**Ce Wang** Tsinghua Univ.	Machine Learning for Frustrated Classical Spin Models
12:15-14:00	*Lunch*	
14:00-14:45	**Giacomo Torlai** Univ. of Waterloo	Neural-Network Quantum State Tomography for Many-Body Systems

14:45-15:30	**Maria Schuld** Kwazulu-Natal	Machine learning with quantum circuits: Constructing a distance-based binary classifier through quantum interference
15:30-16:00	*Break*	
16:00-16:45	**Pan Zhang** ITP, CAS	Mean-field-based spectral method for unsupervised learning: from PCA to non-backtracking and its generalizations
16:45-17:30	**Hai-Ping Huang** RIKEN	Spontaneous symmetry breaking in machine learning: a replica theory
Jul. 5 (Wed.)		
09:00-09:45	**Kieron Burke** UC Irvine	Machine-learning density functionals
09:45-10:30	**Matthias Rupp** FHI Berlin	Unified Representation for Machine Learning of Molecules and Crystals
10:30-11:00	*Break*	
11:00-11:45	**Jun Li** Univ. of Waterloo & CSRC	A Separability-Entanglement Classifier via Machine Learning
11:45-12:15	**Yue-Chi Ma** Tsinghua IIIS	Transforming Bell's Inequalities into State Classifiers with Machine Learning
12:15-14:00	*Lunch*	
14:00-15:30	**Hartmut Neven** Google	[Public Lecture] An Update from the Google Quantum Artificial Intelligence Lab
15:30-16:00	FREE	

Jul. 6 (Thur.)		
09:00-09:45	**Dong-Ling Deng** UMD	Machine learning quantum states and entanglement
09:45-10:30	**Ivan Glasser** MPIQO	The geometry of Neural Network States, String-Bond States and chiral topological order
10:30-11:00	*Break*	
11:00-11:45	**Yi-Chen Huang** Caltech	Neural network representation of tensor network and chiral states
11:45-12:15	**Jing Chen** IOP, CAS	On the Equivalence of Restricted Boltzmann Machines and Tensor Network States
12:15-14:00	*Lunch*	
14:00-14:45	**Jun-Wei Liu** MIT	Self-Learning Monte Carlo Method

14:45-15:15	**Li Huang** CAEP	Accelerated Monte Carlo simulations with restricted Boltzmann machines
15:15-15:45	*Break*	
15:45-16:30	**Miles Stoudenmire** UC Irvine	Machine Learning with Tensor Networks
16:30-18:00	[Rump Session]	
18:00	[Conference Dinner]	

Jul. 7 (Fri.)		
09:00-09:45	**Xiao-Yan Xu** IOP, CAS	Self-Learning quantum Monte Carlo method in interacting fermion systems
09:45-10:15	**Huitao Shen** MIT	Self-learning Monte Carlo Method: Continuous Time Algorithm
10:15-10:45	*Break*	
10:45-11:15	**Nobuyuki Yoshioka** Univ. of Tokyo	Machine Learning Phases of Disordered Topological Superconductors
11:15-11:45	**Satoru Tokuda** AIST	Bayesian spectral deconvolution: How many peaks are there in this spectrum?

Abstract

A Brief Introduction to Machine Learning
Wei-Shan Dong (Baidu Research)

This tutorial aims to provide a brief introduction to the core concepts of machine learning and how machine learning help us solving real-world problems. I will take binary classification as a starting point to introduce the general formulation of supervised learning, and meanwhile, to show the basic ideas of several popular machine learning algorithms, including Support Vector Machines (SVM), Logistic Regression (LR), and Neural Networks (aka Deep Learning). I will also share some experiences of machine learning applications from the industry's point of view.

[Blackboard] Neural-network Quantum States
Giuseppe Carleo (ETH Zurich)

Machine-learning-based approaches are being increasingly adopted in a wide variety of domains, and very recently their effectiveness has been demonstrated also for many-body physics [1-4]. In this seminar I will present recent applications to quantum physics.

First, I will discuss how a systematic machine learning of the many-body wave-function can be realized. This goal has been achieved in [1], introducing a variational representation of quantum states based on artificial neural networks. In conjunction with Monte Carlo schemes, this representation can be used to study both ground-state and unitary dynamics, with controlled accuracy. Moreover, I will show how a similar representation can be used to perform efficient Quantum State Tomography on highly-entangled states [5], previously inaccessible to state-of-the art tomographic approaches.

I will then briefly discuss, recent developments in quantum information theory, concerning the high representational power of neural-network quantum states.

[1] Carleo, and Troyer -- Science 355, 602 (2017).
[2] Carrasquilla, and Melko -- Nat. Physics doi:10.1038/nphys4035 (2017)
[3] Wang -- Phys. Rev. B 94, 195105 (2016)
[4] van Nieuwenburg, Liu, and Huber -- Nat. Physics doi:10.1038/nphys4037 (2017)
[5] Torlai, Mazzola, Carrasquilla, Troyer, Melko, and Carleo -- arXiv:1703.05334 (2017)

A neural network perspective on the Ising gauge theory and the toric code

Juan Carrasquilla (D-Wave System)

I will discuss a supervised learning perspective on the Ising gauge theory and demonstrate potential problems of doing that by constructing adversarial examples that scrutinize the model's ability to sort ground states from excited states. I will show an analytical solution that addresses these issues and will show connections of the solution to the ground state of the toric code.

Quantum Loop Topography for Machine learning on topological phase, phase transitions, and beyond

Frank Yi Zhang (Cornell Univ.)

Despite rapidly growing interest in harnessing machine learning in the study of quantum many-body systems, there has been little success in training neural networks to identify topological phases. The key challenge is in efficiently extracting essential information from the many-body Hamiltonian or wave function and passing the information to a neural network. When targeting topological phases, this task becomes particularly challenging as topological phases are defined in terms of non-local properties. Here we introduce Quantum Loop Topography: a procedure of constructing a multi-dimensional image containing essential information on the phase of the corresponding "sample" Hamiltonian or wave function, by evaluating relevant operators at independent Monte Carlo steps. Such operators take semi-local loop structures, and are determined by either the characteristic responses or the quasi-particle statistics of the targeted phase. Feeding the Quantum Loop Topography into a fully-connected neural network with a single hidden layer, we demonstrate that the architecture can be effectively trained to distinguish Chern insulator and fractional Chern insulator, as well as Z2 quantum spin liquid, with high efficiency and fidelity. Given the versatility of the procedure that can handle different lattice geometries, disorder, interaction and even degeneracy our work paves the route towards powerful applications of machine learning in the study of topological quantum matters, phase transitions, and beyond.

[1] Yi Zhang, Roger G. Melko, and Eun-Ah Kim, arXiv-eprint(2017); Yi Zhang, and Eun-Ah Kim, Phys. Rev. Lett. 118, 216401 (2017) [Editors' Suggestion and Viewpoint].

Machine learning phases of strongly-correlated fermions

Ehsan Khatami (San Jose State Univ.)

Machine learning offers an unprecedented perspective for the problem of classifying phases in condensed matter physics. I will present the first application of neural network machine learning techniques to distinguish finite-temperature phases of the strongly-correlated fermions. I will show that a convolutional network trained on auxiliary field configurations produced by quantum Monte Carlo (QMC) simulations of the 3D Hubbard model can correctly predict the magnetic phase diagram of the model at the average density of one (half filling). I will then discuss a transfer-learning approach in which a network that is trained at half filling can predict the magnetic phase transition away from half filling in the presence of the QMC "sign problem".

Sparse modeling: how to solve the ill-posed problem

Masayuki Ohzeki (Tohoku Univ.)

Lack of information hampers the inference of the explicit appearance from measurements. However, if you solve some optimization problem, you can get the exact answer from less number of measurements. This is an innovative technology known as the compressed sensing by use of the sparseness of the answer. I will talk about the basic concept of the compressed sensing and its application to the various realms of researches. In addition, I will introduce the dictionary learning to obtain the sparse representation of the target. Both of the technologies leads to a revolution on the various fields involved in the measurements. This is the sparse modeling. I will also show our recent contribution to the realm of many-body physics.

Magnetic Phase Transitions and Unsupervised Machine Learning

Richard Scalettar (UC Davis)

We will describe the application of unsupervised machine learning techniques to phase transitions in several classical spin models- the square and triangular-lattice Ising models, the Blume-Capel model, a highly degenerate biquadratic-exchange spin-one Ising (BSI) model, and the 2D XY model. We find that quantified principal components from principal component analysis (PCA) not only allow exploration of different phases and symmetry-breaking, but can distinguish phase transition types and locate critical points. We show that the corresponding weight vectors have a clear physical interpretation, which are particularly interesting in the frustrated models such as the triangular antiferromagnet, where they can point to incipient orders. The failure to capture the 'charge' correlations (vorticity) in the BSI model (XY model) from raw spin configurations point to some of the limitations of PCA. In the second part of the talk, we will show what PCA can distinguish concerning quantum phase transitions in the ground state of the Periodic Anderson and honeycomb lattice Hubbard Hamiltonians.

Machine Learning for Frustrated Classical Spin Models

Ce Wang (Tsinghua Univ.)

In this talk, we will apply the machine learning method to study classical XY model on frustrated lattices, such as triangle lattice and UnionJack lattice. The low temperature phases of these frustrated models exhibit both U(1) and Z2 chiral symmetry breaking, and therefore they are characterized by two order parameters, and consequently, two successive phase transitions as lowering the temperature. By using classical Monte Carlo to generate a large number of data to feed computer, we use methods such as the principle component analysis (PCA) to analyze these data. We find that the PCA method can distinguish all different phases and locate phase transitions, without prior knowledge of order parameters. Our analysis pave a way to machine learning studies of more sophisticated models.

Neural-Network Quantum State Tomography for Many-Body Systems

Giacomo Torlai (Univ. of Waterloo)

The reconstruction of an unknown quantum state from simple experimental measurements, quantum state tomography (QST), is a fundamental tool to investigate complex quantum systems, validate quantum devices and fully exploit quantum resources.

In this talk, I will introduce a novel scheme for QST using machine-learning [1]. The wave-function of an arbitrary many-body system is parametrized with a standard neural network, which is trained on raw data to approximate both the amplitudes and the phases of the target quantum state. This approach allows one to reconstruct highly-entangled states and reproduce challenging quantities, such as entanglement entropy, from simple measurements already available in the experiments. I will show the main features of the "Neural-Network QST" and demonstrate its performances on a variety of examples, ranging from the prototypical W state, to unitary dynamics and ground states of many-body Hamiltonians in one and two dimensions.

[1] G. Torlai, G. Mazzola, J. Carrasquilla, M. Troyer, R. G. Melko and G. Carleo, arXiv:1703:05334

Machine learning with quantum circuits: Constructing a distance-based binary classifier through quantum interference

Maria Schuld (Kwazulu-Natal)

While machine learning is an increasingly popular method to learn about quantum systems, the vice versa approach - using quantum computers to solve machine learning tasks - has also been investigated in recent years. Sometimes referred to as 'quantum-assisted machine learning', the central question is whether quantum information processing can add anything to machine learning research. The most common strategy is to search for speedups by outsourcing the optimization task in well-known learning classical techniques to quantum devices. In this talk I will argue for a different approach which starts with the framework of quantum algorithms to find out what (new) types of learning models quantum circuits naturally give rise to. As a toy example I will present a simple interference circuit that realises a binary classifier by computing distances between data points in parallel. Such a quantum classifier can be implemented on small scale quantum computers available today.

Spontaneous symmetry breaking in machine learning: a replica theory
Hai-Ping Huang (RIKEN)

Learning hidden features in unlabeled training data is called unsupervised learning. Understanding how data size confines learning process is a topic of interest not only in machine learning but also in cognitive neuroscience. The merit of unsupervised feature learning puzzles the community for a long time, and now as deep learning gets popular and powerful, a theoretical basis for unsupervised learning becomes increasingly important but is lacked so far. Our simple statistical mechanics model substantially advances our understanding of how data size confines learning, and opens a new perspective for both neural network training and related statistical physics studies.

Machine-learning density functionals
Kieron Burke (UC Irvine)

I will introduce modern density functional theory and the search for good approximate functionals. I will then discuss two recent works, one in which we do the first ever machine-learned DFT molecular dynamics simulation, and the other in which we show how ML can produce the exact density functional for strongly correlated solids (at least in 1d). All papers/preprints available from http:dft.ps.uci.edu.

A Separability-Entanglement Classifier via Machine Learning
Jun Li (Univ. of Waterloo & CSRC)

The problem of determining whether a given quantum state is entangled lies at the heart of quantum information processing, which is known to be an NP-hard problem in general. Despite the proposed many methods – such as the positive partial transpose (PPT) criterion and the k-symmetric extendibility criterion – to tackle this problem in practice, none of them enables a general, effective solution to the problem even for small dimensions. Explicitly, separable states form a high-dimensional convex set, which exhibits a vastly complicated structure. In this work, we build a new sepaFrability-entanglement classifier underpinned by machine learning techniques. Our method outperforms the existing methods in generic cases in terms of both speed and accuracy, opening up the avenues to explore quantum entanglement via the machine learning approach.

Transforming Bell's Inequalities into State Classifiers with Machine Learning

Yue-Chi Ma (Tsinghua IIIS)

Quantum information science has profoundly changed the ways we understand, store, and process information. A major challenge in this field is to look for an efficient means for classifying quantum states. For instance, one may want to determine if a given quantum state is entangled or not. However, %no effective solution exists for the NP-hard complexity of this problem in general. Moreover, the process of a complete characterization of quantum states, known as quantum state tomography, is a resource-consuming operation. An attractive proposal would be the use of Bell's inequalities as an entanglement witness, where only partial information of the quantum state is needed. The problem is that entanglement is necessary but not sufficient for violating Bell's inequalities, making it an unreliable state classifier. Here we aim at solving this problem by the methods of machine learning. More precisely, given a family of quantum states, we randomly picked a subset of it to construct a quantum-state classifier, accepting only partial information of each quantum state. Our results indicated that these transformed Bell-type inequalities can perform significantly better than the original Bell's inequalities in classifying entangled states. We further extended our analysis to three-qubit and four-qubit systems, performing classification of quantum states into multiple species. These results point to a new direction where machine learning can be utilized for solving practical problems in quantum information science.

[Public Lecture] An Update from the Google Quantum Artificial Intelligence Lab
Hartmut Neven (Google)

In this talk I will report about ongoing efforts at the Google Quantum AI Lab to engineer a processor that is capable of passing the quantum supremacy frontier. This is defined as the moment when a quantum processor becomes capable of executing a computational task in a short time, say one second, while even the fastest classical supercomputer cannot perform this task within a reasonable time frame, say one year. Once the supremacy milestone is achieved we plan to offer access to our quantum processors via Google Cloud for researchers and practitioners to be able to explore their potential computational powers. I will discuss which useful application we hope to run on such near-term quantum processors which have passed the quantum supremacy frontier but do not yet possess enough qubits to perform quantum error correction. I will discuss three application areas: quantum simulation, quantum enhanced optimization and quantum neural networks. In particular I will report on i) a recent breakthrough in quantum simulation that suggests that one only needs a circuit of depth O(n) to perform electronic structure calculations involving n spin orbitals ii) quantum parallel tempering, a newly designed quantum enhanced optimization technique, that uses the physics of many body delocalization to escape local minima and finally iii) first experiments to train quantum neural networks.

Machine learning quantum states and entanglement
Dong-Ling Deng (UMD)

Recently, machine learning has attracted tremendous interest across different communities. In this talk, I will briefly introduce a new neural-network representation of quantum many-body states and show that this representation can describe certain topological states in an exact and efficient fashion. I will talk about the entanglement properties, such as entanglement entropy and spectrum, of those quantum states that can be represented efficiently by neural networks. I will also show that neural networks can be used, through reinforcement learning, to solve a challenging problem of calculating the massively entangled ground state for a model Hamiltonian with long-range interactions.

The geometry of Neural Networks States, String-Bond States and chiral topological order

Ivan Glasser (MPIQO)

Neural Networks Quantum States have been recently introduced as an Ansatz for describing the wave function of strongly correlated quantum many-body systems. We show that fully connected Neural Networks States are String-Bond States with a particular non-local geometry and low bond dimension, while convolutional Neural Networks states are Entangled Plaquette states. This provides a generic way of enhancing the power of Neural Networks State and a natural generalization to systems with larger local Hilbert space. While it remains a challenge to describe states with chiral topological order using traditional Tensor Networks, we show that due to their non-local geometry Neural Networks States can describe exactly a lattice Fractional Quantum Hall state. In addition, we give numerical evidence that Neural Networks States can approximate a chiral spin liquid, where Entangled Plaquette States and local String-Bond States fail. Finally we discuss the limitations of these states and argue that a suitable combination of different classes of states can in general be used to target the ground state of a many-body Hamiltonian.

Neural network representation of tensor network and chiral states

Yi-Chen Huang (Caltech)

We study the representational power of a Boltzmann machine (a type of neural network) in quantum many-body systems. We prove that any (local) tensor network state has a (local) neural network representation. The construction is almost optimal in the sense that the number of parameters in the neural network representation is almost linear in the number of nonzero parameters in the tensor network representation. Despite the difficulty of representing (gapped) chiral topological states with local tensor networks, we construct a quasi-local neural network representation for a chiral p-wave superconductor. This demonstrates the power of Boltzmann machines.

On the Equivalence of Restricted Boltzmann Machines and Tensor Network States

Jing Chen (IOP, CAS)

Restricted Boltzmann machine (RBM) is one of the fundamental building blocks of deep learning. RBM finds wide applications in dimensional reduction, feature extraction, and recommender systems via modeling the probability distributions of a variety of input data including natural images, speech signals, and customer ratings, etc.

We build a bridge between RBM and tensor network states (TNS) widely used in quantum many-body physics research. We devise efficient algorithms to translate an RBM into the commonly used TNS. Conversely, we give sufficient and necessary conditions to determine whether a TNS can be transformed into an RBM of given architectures. Revealing these general and constructive connections can cross-fertilize both deep learning and quantum-many body physics. Notably, by exploiting the entanglement entropy bound of TNS, we can rigorously quantify the expressive power of RBM on complex datasets. The discussion of different topological sectors of toric code can be directly applied to RBM. Insights into TNS and its entanglement capacity can guide the design of more powerful deep learning architectures. On the other hand, RBM can represent quantum many-body states with fewer parameters compared to TNS, which may allow more efficient classical simulations. It is interesting that entanglement is not the only issue to represent RBM of TNS, such as AKLT. With the bridge, we also find that the shift-invariant RBM [5] increases the expressive power of entanglement.

Other three works "Quantum Entanglement in Neural Network States" [2] and "Efficient Representation of Quantum Many-body States with Deep Neural Networks"[3], "Neural network representation of tensor network and chiral states" [4] will be also talked about. These four papers have some overlaps but from different view angles.

[1]J. Chen, S. Cheng, H. Xie, L. Wang, and T. Xiang, arXiv:1701.04831 [Cond-Mat, Physics:quant-Ph, Stat] (2017).
[2]D.-L. Deng, X. Li, and S. D. Sarma, arXiv:1701.04844 [Cond-Mat, Physics:quant-Ph] (2017).
[3]X. Gao and L.-M. Duan, arXiv:1701.05039 [Cond-Mat, Physics:quant-Ph] (2017).
[4]Y. Huang and J. E. Moore, arXiv:1701.06246 [Cond-Mat] (2017).
[5]G. Carleo and M. Troyer, Science 355, 602 (2017).

Accelerated Monte Carlo simulations with restricted Boltzmann machines
Li Huang (CAEP)

Despite their exceptional flexibility and popularity, Monte Carlo methods often suffer from slow mixing times for challenging statistical physics problems. We present a general strategy to overcome this difficulty by adopting ideas and techniques from the machine learning community. We fit the unnormalized probability of the physical model to a feed-forward neural network and reinterpret the architecture as a restricted Boltzmann machine. Then, exploiting its feature detection ability, we utilize the restricted Boltzmann machine to propose efficient Monte Carlo updates to speed up the simulation of the original physical system. We implement these ideas for the Falicov-Kimball model and demonstrate an improved acceptance ratio and autocorrelation time near the phase transition point.

Machine Learning with Tensor Networks
Miles Stoudenmire (UC Irvine)

The development of tensor network descriptions of quantum wavefunctions has been a crucial advance in physics, leading to controlled algorithms for computing properties of quantum many-body systems and rigorous insights into subtle phases of matter. But tensor networks are actually a very general tool, and can in principle be applied to many problems outside of physics too.

I will describe a way to use tensor networks to parameterize certain machine learning models, related to kernel learning and support vector machines. Specializing to matrix product state networks yields an training algorithm scaling significantly better than previous methods for similar models. I will discuss some new results on initializing these models and applying them to larger input spaces. Finally, I will discuss connections to related ideas in the machine learning literature and discuss future insights that tensor networks could provide.

Self-Learning quantum Monte Carlo method in interacting fermion systems

Xiao-Yan Xu (IOP, CAS)

Self-learning Monte Carlo method is a powerful general-purpose numerical method recently introduced to simulate many-body systems. In this work, we extend it to interacting fermion quantum system in the framework of widely used determinantal quantum Monte Carlo. The new method can generally reduce the computational complexity, and moreover can greatly reduce the autocorrelation time near a critical point. This enables us to simulate interacting fermion system on a 100×100 lattice even at the critical point for the first time, and obtain critical exponents with high precision.

Machine Learning Phases of Disordered Topological Superconductors

Nobuyuki Yoshioka (Univ. of Tokyo)

A topological superconductor (TSC) is a superconductor (SC) with a bulk gap characterized by a nontrivial topological invariant, which reflects the global property of the wave functions [1]. While the concrete expression of the topological number for the translationally invariant system is widely known, our understanding of the disordered SCs is limited. In this work, we investigate the phases of two-dimensional disordered TSC in the class DIII using the state-of-the-art machine learning technique which outperforms other methods in image recognition, i.e., the convolutional neural network (CNN) [2].

With the surging development of experimental research, there is a growing demand for investigation in the class DIII system, or the spin-rotation-symmetry-breaking Bogoliubov de Gennes system with time reversal symmetry, since some candidate materials are believed to belong here (e.g. CuxBi2Se3, FeTexSe1-x). There are two valid ways to model such systems. One is so-called Chalker-Coddington network model [3], which phenomenologically formulates the propagation and the scattering of the electrons. The other method we consider in this work is the tight-binding model, whose parameters re ect the microscopic information and hence expected to be in a good connection with experimental works. The Z 2 topological invariant exhibited in this class is re ected in the real-space distribution of the quasiparticle according to the bulk-edge correspondence. Hence, we give the machine the distribution as a "picture" with some label to learn the structure and perform the supervised learning [4,5]. In our presentation, we compare the result to the phase diagram obtained by other methods (See Fig. 1), namely the transfer matrix and non-commutative geometry [6], and discuss the accuracy and the validity of the new technique

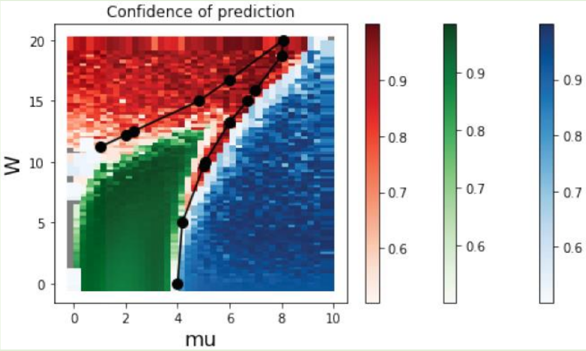

Figure 1: Phase diagram of helical superconductor with disorder. The red, green and blue regions denote thermal metal, topological, and trivial states, respectively, and their depth correspond to the confidence of the machine.

[1] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
[2] Y. LeCun, Y. Bengio, and G. Hinton, Nature 521, 436 (2015).
[3] I. C. Fulga et al., Phys. Rev. B 86, 054505 (2012).
[4] T. Ohtsuki and T. Ohtsuki, J. Phys. Soc. Jpn 85, 123706, (2016).
[5] T. Ohtsuki and T. Ohstuki, J. Phys. Soc. Jpn 86, 044708 (2016).
[6] H. Katsura and T. Koma, arXiv:1611.01928 (2016).

Bayesian spectral deconvolution: How many peaks are there in this spectrum?

Satoru Tokuda (AIST)

There is a fundamental problem in identifying the peaks in noisy complex spectra: How many peaks are there in this spectrum? We propose a framework based on Bayesian inference, which enables us to separate multipeak spectra into the appropriate single peaks statistically. Our framework efficiently enables us to seek not just global minima solutions of fitting parameters of each peak function to the given spectrum but also local minima solutions by using the exchange Monte Carlo (EMC) method. In addition, we can also calculate Bayesian free energy, which is a criterion of the appropriate peak number and the noise level, because seeking the fitting parameter by the EMC method is regarded as sampling from the probability density of the fitting parameter. In our presentation, we demonstrate how efficient our framework is and also discuss the inseparability of the peak number and the noise level in Bayesian inference, based on the relationship between Bayesian inference and statistical physics.

Contact List

Note: The contact information is provided for the convenience of attendees to collaborate and keep in touch. This information should not be shared with non-registered attendees and please respect the privacy of other attendees by not compiling this list for the purpose of sending unsolicited emails, or by sharing personal information without approval. Thank you.

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