DLAP2019 Poster title and abstract

Nagai, Yuki (Japan Atomic Energy Agency)

Self-learning Hybrid Monte Carlo for first-principles molecular simulations

We propose a novel approach called Self-Learning Hybrid Monte Carlo (SLHMC)[1] which is a general method to make use of machine learning potentials to accelerate the statistical sampling of first-principles density-functional-theory (DFT) simulations. The trajectories are generated on an approximate machine learning (ML) potential energy surface. The trajectories are then accepted or rejected by the Metropolis algorithm based on DFT energies. In this way the statistical ensemble is sampled exactly at the DFT level for a given thermodynamic condition. Meanwhile the ML potential is improved on the fly by training to enhance the sampling, whereby the training data set, which is sampled from the exact ensemble, is created automatically.

[1]Yuki Nagai, Masahiko Okumura, Keita Kobayashi, and Motoyuki Shiga, arXiv:1909.02255

Shirai, Tatsuhiko (Green Computing Systems Research Organization, Waseda University)

Generalized quantum annealing inspired by thermal effect

With the progress of quantum technology, it is becoming essential for exploring the potential of Ising machines in the field of machine learning. Ising machines provide heuristic solvers for a combinatorial optimization problem, which is ubiquitous in the whole procedure of machine learning. Toward the realization of more efficient solvers, in this poster, we propose a generalized quantum annealing method inspired by a thermal effect. We present an influence of the thermal effect on the performance and evaluate the fair sampling of the degenerate ground states.

Tamura, Kensuke (Department of Physics, Graduate School of Science, The University of Tokyo)

Performance comparison of integer encoding methods in Ising machines

Combinatorial optimization problems have wide applications in various fields including machine learning. These problems can be mapped to finding the ground states of the corresponding classical Ising model, which can be solved efficiently by Ising machines. Recently, potential applications of Ising machines to machine learning have been explored. Toward the realization of high-performance machine learning by using Ising machines, we need to rephrase optimization procedures in machine learning as combinatorial optimization problems, which have to be described by binary variables, i.e., {0,1}. To this end, it is convenient to use integer encodings which converts any integer into a binary string. There are four typical integer encodings: one-hot, log, unary and order encoding and it is important to clarify which of these methods performs better. In this poster presentation, we compare these four methods for 0-1 quadratic knapsack problems using an Ising machine.

Seryo, Naoki (Department of Chemical Engineering, Kyoto University)

Learning constitutive relations from micro-scale dynamics with memory effects in non-Newtonian fluids

Polymeric materials, which are widely used in industry, are usually created from polymer melts. These melts are an example of a complex fluid, where the behavior is determined by the microscopic dynamics of the entangled polymer chains. For this reason, the mechanical properties and the flow state of the polymer melt are extremely complicated. Therefore, to reliably control the nature of the flow and the degree of entanglement, detailed simulations are required. However, performing microscopic simulations is out of the questions, given the large separation of length- and time-scales between the microscopic and macroscopic degrees of freedom. Therefore, to deal with the relationship between micro-scale and macro-scale in detail, Multi-Scale Simulations (MSS) of polymeric fluids have become the standard approach. Unfortunately, this still

requires considerable computational resources. This study aims to develop a data-driven multi-scale simulation method to derive the constitutive relation of non-Newtonian fluids exhibiting memory effects. For this, we introduce a Gaussian Process Regression model to derive the constitutive relation from the microscopic simulation. This allows us to drastically reduce the calculation cost, compared to full MSS. To test our method, we consider the case of simple shear flow with a Hookean-dumbbell model for the polymer chains. Our results in excellent agreement with the MSS and offer the possibility of deriving the constitutive relations for more complicated microscopic polymer models.

Mototake, Yoh-ichi (The Institute of Statistical Mathematics)

Conservation Law Estimation by Extracting the Symmetry of a Dynamical System Using a DNN

From the viewpoint that Deep Neural Networks (DNN) have the ability to model the distribution of dataset as a low-dimensional manifold, we propose a method to extract the coordinate transformation making a dataset distribution invariant by sampling DNN using Replica Exchange Monte-Carlo method. In addition, we show that the canonical transformation that makes the Hamiltonian invariant, which is necessary condition for Noether's theorem, and symmetry of the manifold structure of the time series data of the dynamical system are related.
By integrating this knowledge with the method described above, we propose a method to estimate conservation law from time-series data.
We verified the efficiency of the proposed methods in some primitive cases.

Berns, Lukas (Tokyo Institute of Technology)

A new CNN architecture for sub-manifolds embedded into higher dimensional space

We study methods to overcome practical challenges in applying CNNs to water Cherenkov detectors like Super-Kamiokande. Here a huge volume of water is

surrounded by light detectors, which record the hit position and timing of photons emitted from relativistic particles inside the tank. The task is particle ID and reconstruction of track parameters like energy or interaction vertex. We propose a way to apply a CNN to the 2D sub-manifold formed by the light detectors, that correctly takes into account the S_2 topology, as well as the reparametrization invariance of the sub-manifold coordinates. In our formulation the integration kernels have a geometrical interpretation, which can be utilized to enlarge the intrinsic translation symmetry in 3D space by rotational symmetry. These features make the network robust against overtraining, suggesting the possibility for data-driven training at the small sample sizes of neutrino events.

Matsumoto, Ryo (Tokyo University of Science)

Classification of Super-Kamiokande atmospheric neutrino events by using neural network

Neutrino mass hierarchy (MH) is not yet determined while it was revealed from observation of neutrino oscillation that the extremely small neutrino mass exists. Current precision of MH in Super-Kamionade is limited by the statistics in a few GeV region where resonance oscillation occurs due to Earth's matter effects. In this study, we investigated a classification of multi-GeV multi-ring events by neural network. We will present the evaluation of the method using the atmospheric neutrino MC simulations.

Yoshioka, Nobuyuki (Department of Physics, University of Tokyo)

Constructing neural stationary states for open quantum many-body systems

We propose a new variational scheme based on the neural-network quantum states to simulate the stationary states of open quantum many-body systems. Using the high expressive power of the variational ansatz described by the restricted Boltzmann machines, which we dub as the neural stationary state

ansatz, we compute the stationary states of quantum dynamics obeying the Lindblad master equations. The mapping of the stationary-state search problem into finding a zero-energy ground state of an appropriate Hermitian operator allows us to apply the conventional variational Monte Carlo method for the optimization. Our method is shown to simulate various spin systems efficiently, i.e., the transverse-field Ising models in both one and two dimensions and the XYZ model in one dimension.

Sumimoto, Takayuki (Osaka University)

Meson Spectrum in Holographic QCD and Deep Learning

In my talk, I will report that 5d theory on curved spacetime describing the meson spectrum was found by using deep learning. Based on holographic principle, we employed deep learning as a method obtaining bulk geometry dual to a certain QFT. Our input data was the spectrum of meson, QCD observables. Then experimental data of spectrum gave the metric of bulk spacetime as learning weight of neural network. I will explain about how the bulk spacetime emerged on neural network and discuss its consistency as bulk spacetime dual to QCD.

Lim, Sung Hak (Theory Center, HIGH ENERGY ACCELERATOR RESEARCH ORGANIZATION, KEK)

Interpretable deep learning for two-prong jet classification with jet spectra

Classification of jets with deep learning has gained significant attention in recent times. However, the performance of deep neural networks is often achieved at the cost of interpretability. Here we propose an interpretable network trained on the jet spectrum S2(R) which is a two-point correlation function of the jet constituents. The spectrum can be derived from a functional Taylor series of an arbitrary jet classifier function of energy flows. An interpretable network can be obtained by truncating the series. The intermediate feature of the network is an infrared and collinear safe C-correlator which allows us to estimate the

importance of an S2(R) deposit at an angular scale R in the classification. The performance of the architecture is comparable to that of a convolutional neural network (CNN) trained on jet images, although the number of inputs and complexity of the architecture is significantly simpler than the CNN classifier. We consider two examples: one is the classification of two-prong jets which differ in color charge of the mother particle, and the other is a comparison between Pythia 8 and Herwig 7 generated jets.

Shiina, Kenta (Department of Physics, Tokyo Metropolitan University)

Solving Schrodinger equation by Machine Learning with support of Perturbation theory

We tried to make Neural network (NN) learn the mapping between a potential energy and its wave function for time-independent system. Unlike previous studies, we don't prepare any exact solutions (ground truth) provided by other numerical methods. Instead of that, we use first perturbation of wave function as supportive information in order to help NN learn the mapping. We found that trained NN can produce an approximated wave function for new input of potential energy which is not included in training data. The advantages of our method are that it doesn't require ground truth as training data set, and it can be applied to any quantum state if the first perturbation of target state can be calculated.

Kuriki, Ryosuke (Tokyo University of Science)

Deep learning method to solve an inverse problem clarifying the properties of thermoelectric materials from observables

Thermoelectric effects are typical phenomena in material physics. They are attracting much attention from the viewpoint of energy harvesting. Recently, Yamamoto and Fukuyama clarified their theoretical structures using Kubo formula. In their frameworks, electrical conductivity and thermoelectrical

conductivity are given by fermi-distribution and spectrum conductivity. This spectrum conductivity depends on the physics of target materials, that is, we need to know its behavior to find the origin of thermoelectric effects of the materials, However, spectrum conductivity is not observable while we can measure the electrical conductivity are thermoelectric conductivity. The relation between electrical conductivity (or thermoelectric conductivity) and spectrum conductivity is shown in Fredholm integral equation(FIE). The problem to solve FIE is a kind of inverse problem. Thus, in the present study, we tried to solve this FIE using Deep learning. In our presentation, we show that the spectrum conductivity can be estimated by electrical conductivity and thermoelectric conductivity in some typical cases. Furthermore, we discuss how to apply the present method to real measurements.

Ota, Toshihiro (Osaka University)

Robust and Transferable Adversarial Examples from Deep Image Prior

The accuracy of image recognition using machine learning is already beyond human-level. However, it has been known that a trained neural net is easily fooled by a tiny perturbation, which is called an adversarial example. To study the vulnerability of neural nets, we focus on VGG16, a trained convolutional neural net, and explore how we can deceive the network by making a perturbation through another neural net, deep image prior. In our setup, unlike the normal method, we train deep image prior to cheat VGG16 more efficiently, and it turns out that our noise images show transferability. From our result, we conclude that adversarial example may be extracting a universal concept rather than attacking.

Mano, Tomohiro (Department of Physics, Sophia University)

Application of convolutional neural network to quantum percolations in topological systems

Quantum material phases such Anderson insulator, diffusive metal, Weyl/Dirac semimetal as well as topological insulators show specific wave functions both in real and Fourier spaces. These features are well captured by convolutional neural networks, and the phase diagrams have been obtained, where standard methods are not applicable. One of the examples are the cases of random lattices such as quantum percolation. Here we study the topological insulators with random vacancies, namely the quantum percolation in topological insulators, by analyzing the wave functions via convolutional neural network. The vacancies in topological insulators are especially interesting since peculiar bound states are formed around the vacancies. We show that only a few percent of vacancies derives topological phase transition. The results are confirmed by density of states and wave packet dynamics.

Robles, Sandra (The University of Melbourne)

A deep learning approach to halo merger tree construction

Semi-analytic models for galaxy formation are best suited to compare theories with observations. These models rely heavily on halo merger trees which encapsulate the growth and merger history of dark matter (DM) halos. Despite being computationally intensive, the most popular method for merger tree construction is based on high-resolution DM only N-body simulations. With the aim to provide a new framework for halo merger tree construction with a modest computational cost, we propose a Generative Adversarial Network (GAN) that learns to generate realistic halo merger trees taking advantage of the results of large volume simulations. We train our GAN with merger trees from the EAGLE simulation suite, and show the quality of our results.

Hayase, Tomohiro (Fujitsu Laboratories LTD)

Free Probability Theory for Jacobian Spectrum of Neural Networks

Motivated by the hypothesis that well-conditioned Jacobian spectrum can speed up learning of deep neural networks, Pennington, Sonenholtz, and Ganguli introduced a spectral analysis of the Jacobian with mean-field approximation.
Based on Free probability theory, it is revealed that how the asymptotic spectral distribution of the Jacobian of deep networks depend on initialization of weights and activation functions.
This poster introduces how to guarantee the analysis of the Jacobian mathematically.

Kudo, Kazue (Department of Computer Science, Ochanomizu University)

Constrained quantum annealing of graph coloring

We investigate an efficient quantum annealing approach based on real-time quantum dynamics for graph coloring. The total Hamiltonian consists of driving and problem Hamiltonians. In the constrained quantum annealing, a driving Hamiltonian is chosen so that constraints are naturally satisfied without penalty terms and the dimension of the Hilbert space is considerably reduced. Real-time quantum simulations in a small system provide some insight into quantum annealing.

Nomura, Yusuke (RIKEN Center for Emergent Matter Science)

Machine learning reveals nodal spin liquid in S=1/2 J1-J2 Heisenberg model on square lattice

We study the phase diagram of S=1/2 J1-J2 Heisenberg model on square lattice by using machine learning variational methods. We show that the combination of restricted Boltzmann machine and pair-product wave function gives highly accurate description of the quantum states. We find that there exist nodal spin liquid ground state in the S=1/2 J1-J2 Heisenberg model.

Kitazawa, Masakiyo (Physics, Osaka University)

Deep learning topological sector in lattice gauge theory

We apply a machine learning technique for identifying the topological charge of quantum gauge configurations in four-dimensional SU(3) Yang-Mills theory. The topological charge density measured on the original and smoothed gauge configurations with and without dimensional reduction is used for inputs of the neural networks (NN) with and without convolutional layers.

Huebsch, Marie-Therese (Graduate School of Frontier Sciences, University of Tokyo)

Towards a Feature Space for Magnetic Structures

Many calculations in solid state physics become dramatically more efficient by using an orthonormal basis adapted to the symmetry of the material. The cluster multipole (CMP) expansion for magnetic structures [1] provides an orthonormal basis set of magnetic configurations based on the crystallographic point group. Recent discussions in terms of CMPs established a novel perspective on transverse response properties [2] and spin dynamics in non-collinear antiferromagnets [3]. Our analysis of the experimental data found on MagnData provided by Bilbao Crystallographic Server [4] suggests that only a few terms are finite in the CMP expansion of the most stable configurations in nature. This sparseness can be exploited to build a larger learning database, however that is provided that a reliable prediction of the most stable configuration can be made?possibly by means of ab-initio calculations.

[1] M.-T. Suzuki et al., Phys. Rev. B 99, 174407 (2019).

[2] M. Ikhlas et al., Nat. Physics volume 13, pages 1085-1090 (2017); T. Higo et al., Nat. Photonics 12, 73?78 (2018).

[3] T. Nomoto and R. Arita, arXiv:1903.02259.

[4] S. V. Gallego et al., J. Appl. Cryst. 49, 1941-1956 (2016).

Tanabe, Takehiko (National Metrology Institute of Japan, National Institute of Advanced Industrial Science and Technology)

Potential for improving the local realization of coordinated universal time with a convolutional neural network

The time difference between coordinated universal time (UTC) and a hydrogen maser, which is a master oscillator for the local realization of UTC at the National Metrology Institute of Japan (UTC(NMIJ)), has been predicted by using a one-dimensional convolutional neural network (1D-CNN). We have found that the present 1D-CNN shows better performance as a predictor compared to that based on the Kalman filter, which suggests that the new computational approach may provide a new and useful method for improving the synchronous accuracy of UTC(NMIJ) relative to UTC.

Hayashi, Yusuke (Japan Digital Design Inc.)

Neural Demon: Maxwell's demon as a meta-learner

In recent years, deep learning has achieved remarkable success in supervised and reinforcement learning problems, such as image classification, speech recognition, and game playing. However, these models are specialized for the single task they are trained for. Meta-learning or few-shot learning offers a potential solution to this problem: by learning to learn across data from multiple previous tasks, few-shot meta-learning algorithms can discover the structure among tasks to enable fast learning of new tasks. In this presentation, we consider a hierarchical Bayesian model with a global latent variable θ and task-specific latent variables φ={φ^(t)}. First, we show that when the distribution of latent variables in the decoder p(θ, φ) is equal to the marginal distribution of the encoder q(θ, φ), the thermodynamic costs of the meta-learning process provide an upper bound on the amount of information that the model is able to learn from its teacher. This allows us to introduce the second law of information thermodynamics on meta-learning. Next, we propose the application of this model to multi-task image classification.

Konno, Tomohiko (National Institute of Information and Communications Technologies)

Deep Learning Model for Finding New Superconductors

Superconductivity has been extensively studied since its discovery in 1911. However, the feasibility of room-temperature superconductivity is unknown. There is no theory of high-temperature superconductors and there are no computational methods for strongly correlated systems, in which high-temperature superconductivity emerges. Exploration of new superconductors still relies on the experience and intuition of experts and is largely a process of experimental trial and error. In one study, only 3% of the candidate materials showed superconductivity. Here we report an interdisciplinary attempt for finding new superconductors based on deep learning. We represented the periodic table in a way that allows a deep learning model to learn it. Although we used only the chemical composition of materials as information, we obtained an R-squared value of 0.92 for predicting the superconducting transition temperature, Tc, for materials in a database of superconductors. We obtained three remarkable results. The deep learning method can predict superconductivity for a material with a precision of 62%, which shows the usefulness of the model; it found the recently discovered superconductor CaBi2, which is not in the superconductor database; and it found Fe-based high-temperature superconductors (discovered in 2008) from the training data before 2008. These results open the way for the discovery of new high-temperature superconductor families.

Neupane, Chetanath (Tribhuvan University, Nepal)

Machine learning based study and visualization of molecular dynamics of oxymyoglobin protein using PyMOL and UCSF Chimera

PyMOL and UCSF Chimera are molecular visualization tools, which have been developed to provide clear image in molecular dynamic simulation of proteins and other similar complex biostructures. Using these tools we can visualize three-dimensional structures of bio-molecules graphically to understand the complete structural sketch of biological phenomena elegantly.

In this work, we study necessary numerical techniques and algorithms for the analysis to numerically integrate Newton's equation of motions needed for molecular dynamics simulations. We have taken oxymyoglobin protein for which the required protein file is PDB ID 1MBO.pdb as to provide its brief structural details using PyMOL and UCSF Chimera tools. Through the visualization options in both tools, we have found that the iron core of the heme (HEM) group in oxymyoglobin bounds oxygen. Also, using the structure analysis feature of UCSF Chimera, we have estimated the distance between iron core of HEM to the molecular oxygen and the distance between iron core to the histidine 93(H93) and found to be 1.827 A (OXY-iron core) and 2.065A (histidine 93-iron) respectively.

Inubushi, Masanobu (Graduate School of Engineering Science, Osaka University)

Inference of the energy dissipation rate of turbulence by reservoir computing

The dissipation rate of the kinetic energy of fluid motion is the central quantity in the statistical theories and modelings of turbulence. A type of recurrent neural network, called reservoir computing, enables us to accurately infer the energy dissipation rate based only on the kinetic energy. Furthermore, we show that 'reusing' the reservoir computer learned with data at a low Reynolds number is effective for inference of the dissipation rate at much higher Reynolds numbers.

Sakamoto, Kotaro (Center for Computational Sciences, University of Tsukuba)

Towards a geometrical understanding of physical phenomena via extraction of data manifolds using a GAN

Deep generative models learn a mapping from low-dimensional latent spaces to high-dimensional data spaces. Such mapping functions parameterise an immersed manifold in the data space. We investigate GANs for modelling physical data to extract data manifold structure of time series data and report some results.

(Collaboration with Yuichiro Mori and Yoh-ichiro Mototake)