PROCEEDINGS OF SCIENCE

Deep Learning for inverse problems in nuclear physics

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In this talk, I explained the usage of deep learning paradigm into inverse problems solving in high energy nuclear physics, focusing on studies about QCD matter in extreme conditions. To allow for efficient inverse problem solving, well-developed physical priors would be helpful in the solving procedure. Specifically, I introduced two examples with two different strategies involved: one is about QCD transition type identification in heavy ion collisions using supervised learning, where the physics prior is embedded in the training data generated by state-of-the-art model simulations; the other is about effective in-medium heavy quark potential reconstruction based upon lattice QCD data for Bottomonium mass and width, here the prior is manifested inside our devised approach to couple deep neural network represented potential with the Schrödinger equations.

FAIR next generation scientists - 7th Edition Workshop (FAIRness2022)
23-27 May 2022
Paralia (Pieria, Greece)

*Speaker

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1. Introduction

QCD predicts that normal nuclear matter under extreme conditions (high temperature or density) would turn to a new state of matter – the quark gluon plasma (QGP). It's still an popular yet unresolved topic in high energy and nuclear physics to understand the properties of such hot and dense QCD matter. The understanding of extreme QCD matter properties is also relevant to cosmology study, since the whole universe lied in the QGP state a few microseconds after the Big-Bang. Terrestrially a way to explore this new state of nuclear matter in laboratory is Heavy ion collisions (HIC) experiment[1]. At vanishing or small baryon density, the first principle lattice QCD studies show that the normal hadronic matter will smoothly become QGP in cross over manner along with increasing temperature[2]. However, when it comes to finite density region, the QCD phase diagram remains challenging since the involved sign-problem in lattice QCD sector[3], and we have to resort to experiment exploration or other effective theory. Since the involved complexities, data- and computation-intensive features for many of the related studies, new paradigm from deep learning can provide us efficient power-assistance in tackling some of the calculation barrier.

In this talk I take two examples to demonstrate the deep learning based paradigm for inverse problem solving in the exploration of QCD matter in extreme conditions, and conclude the involved strategies for general inverse problems we may encounter.

2. Example 1: identifying hot matter EoS from collision experiment

The first example is about recognizing QCD matter bulk properties from heavy ion collision experiments using supervised learning. The heavy ion collisions provide unique chance on the earth to potentially create and study the extreme state of QCD matter, where the formed QGP however can only exist transiently in early stage of the collision. Due to the fast expansion and cooling down, the "cooked" hot and dense "soup", QGP, will then quickly experience confinement transition. Therefore in experiment what can only be resolved are those finally emitted hadrons or their decay products, with their identify and momentum information can be detected. There we have no direct access to the probably formed QGP state in early time. Furthermore, theoretically we have many uncertainties to be involved in even the state-of-the-art models of heavy ion collision simulation, e.g., initial fluctuations, hot matter's bulk and transport coefficients (e.g., shear or bulk viscosity), freeze-out procedure, later stage hadronic scattering setup, etc. From model simulations it's shown that these different physics factors can have entangled influence on different experimental observables, like particle spectra, yields or their anisotropic collective flows. The conventional way in extracting the involved physics parameters usually rely on trial and error in bringing model simulations with guesstimate of those physical parameters to confront experimental data. It remains challenging to efficiently disentangle different factors and reveal the fundamental physics from the final state measurements in experiments.

In Ref[4] we made an exploratory study to use state-of-the-art deep learning algorithms to directly connect the QCD bulk properties and final state raw information from heavy ion collisions. The evolution of hot and dense QCD matter formed in heavy ion collisions can be well described by 2nd-order dissipative hydrodynamics. The event-by-event relativistic hydrodynamic modelling package, CLVisc [5], is deployed to generate final state pion's spectra in heavy ion collisions, and being implemented different equation of states especially different QCD transition type (cross over, or first order) embedded. With the prepared training data, convolutional neural network (CNN) based model is developed to take the final state spectra as input and trained to predict the class identity of the QCD transition in the used EoS in the corresponding collision event. For the testing we generated two groups of data-set, one from iEBE-VISHNU [6] event-by-event hydrodynamic simulation with MC-Glauber initial condition, the other still from CLVisc simulation with totally different IP-Glasma-like initial condition. In all the involved data set generation, different set up for η/s, τ_0 and freeze-out temperature are implemented to introduce diversity and hopefully make the learned mapping more robust. We showed that the trained CNN gives high prediction accuracies - **on average larger than** 95% - in the testing stage, which is independent of the used initial condition and robust against shear viscosity and other set-ups. We further deepened this strategy by including more realistic consideration then, for example to take into account the afterburner hadronic rescattering, to consider non-equilibrium phase transition, and develop point-net based models to confront the realistic detector readout (hits or tracks of the particles).

3. Example 2: reconstruct in-medium HQ interaction from LQCD data

The second example is about decoding physics of the QCD medium effects on Bottomonium[7] based on lattice QCD measurements. Specifically we investigated the effective heavy quark potential from lattice QCD measured in-medium spectroscopy (mass and width) for Bottomonium, to whom the suppression of production rates in heavy ion collisions has long been taken as a smoking-gun for the QGP formation[8, 9]. Indeed, generally the heavy quarkonium provide a well-calibrated “QCD Force”, to whom the vacuum properties can be reproduced accurately with a Cornell-like potential as baseline for further spot medium modifications. Because of the large mass and relatively small velocity of heavy quarks, potential descriptions within Schrödinger equation are often employed. When it is put inside the QGP medium, first the Color screening effects can happen to weaken the interaction between the two heavy quarks. Furthermore, which is also demonstrated more and more in recent effective field theory studies [10], the interaction potential for the heavy quark bound state can also develop an imaginary part manifested as finite width.

Most of the phenomenology modelling of quarkonium production in HIC all call for knowledge of their in-medium potential to be taken as input. Theoretically, only at very high temperature we have guidance from perturbative QCD calculation based on Hard-Thermal Loop (HTL) for the understanding of in-medium heavy quark potential. Recently lattice QCD released the newly calculation of Bottomonium mass and width at different temperatures [11]. We found that the existing HTL potential on the market can not reproduce these lattice results by varying the screening mass in these expressions. Therefore a model-independent method to reconstruct the heavy quark in-medium potential from the lattice measured spectroscopy is in urgent need.

We introduce two deep neural networks (DNN) to represent the complex-valued heavy quark potential (one for the real part and the other for the imaginary part), and couple them to the solving of the Schrödinger equation to convert the potential into in-medium mass and thermal widths of Bottomonium. These outputs can thus be compared to the lattice results to further guide the tuning on potential to well describe the data. In evaluating the derivative of the objective with respect to potential, the Hellmann-Feynman theorem can be applied where the needed wave

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function is obtained in the forward Schrödinger equation solving procedure. Then gradient based optimization is performed using the evaluated derivatives. After closure tests to validate the method, we reconstructed the temperature and distance dependent potential which reproduce simultaneously the mass and thermal width from lattice QCD data, **with the corresponding χ^2-per-data-point to be 16.5/30**, both the mass and thermal width got simultaneous reproduction. Further, the uncertainty being associated with the reconstructed potential is quantified using Bayesian perspective.

4. Summary: Inverse Problem solving strategies with Deep Learning

Let's summarize technically the above introduced two projects in general manner. There are actually many challenging inverse problems in nuclear physics and also other research areas, where, the forward modeling is straightforward and achievable, while the corresponding inverse process is implicit and might hindered from direct derivation or evaluation, see Fig. 1. Like the above introduced examples, that, it's challenging to inverse the heavy ion collision process to infer the hot matter EoS or inverse the Schrödinger system to reconstruct heavy quark in-medium potential. Some other examples see, e.g., inferring neutron star equation of state from their mass-radius astronomy observations[12], reconstructing spectral function based on Euclidean correlator estimation from Monte Carlo simulation[13], identifying CME in heavy ion collisions[14].

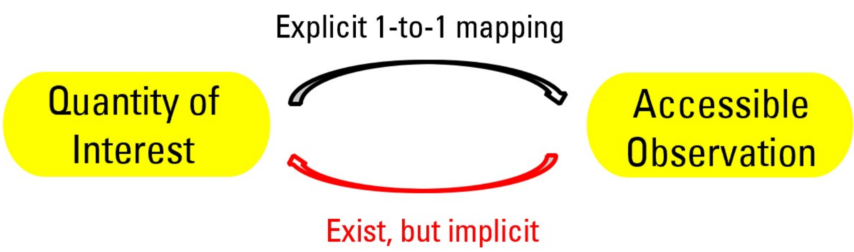

Figure 1: A schematic plot of inverse problems with direct forward models but implicit inverse processes.

With deep learning paradigm, we devised two different strategies in solving such inverse problems from supervised and unsupervised learning perspectives, respectively, where physics priors are also implemented in different manners.

1. The first is supervised learning by preparing training data-set from the forward modeling, with different target parameters values varying and their corresponding observables simulated. Then the direct inverse mapping from observables to the utilized physics parameters can be learned in big-data sense. In Ref.[4, 12, 15, 16] we showed this strategy can well bridge the collision experiment to theory in exploring the involved physics for extreme QCD matter.

2. The second approach applies differentiable programming strategy to perform variation on the target physics parameters (or continuous functions) using gradient-based guidance for the forward modeling. Meanwhile, the target physics can be represented by a deep neural network (DNN) to introduce unbiased but flexible enough parameterization. The objective of the

inference is similar to the conventional χ^2 fitting, thus the difference between the output from forward modeling and the real measurements weighted by observable uncertainties. Using automatic differentiation or linear response analysis it is achievable to evaluate the derivative of the objective with respect to every parameters in the target physics representation, and the optimization will then be possible via gradient descent. Alternatively, heuristic algorithms or Markov-chain Monte Carlo can be employed as well for the inference process.

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